ANALYSIS OF THE POTENTIAL FOR PLANT UPTAKE OF TRICHLOROETHYLENE AND AN ASSESSMENT OF THE RELATIVE RISK FROM DIFFERENT CROP TYPES

THESIS

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AFIT/GEE/ENV/94S-01

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THESIS

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Preface

The purpose of this study was to analyze the potential for plant uptake of trichloroethylene (TCE) and to assess the relative risk from different crop types. The work incorporated three distinct phases. First, a physicochemical screening of TCE, based on relationships reported in previous research, was done to evaluate its potential for uptake by plants. Next, a computerized model of plant uptake processes, specifically the PLANTX model developed by Trapp and others, was used to derive the soil TCE concentrations which would result in plant compartment (i.e., root, stem, leaf, and fruit) levels exceeding the Safe Drinking Water Act maximum concentration level of five micrograms per liter (1990). Information from both approaches was then used to determine the likely locations in plants where accumulation of TCE may be of concern to human health. Finally, the above procedures were applied to an existing TCE contamination situation at Hill Air Force Base near Ogden, Utah.

Without the support and guidance of others, this work would not have been possible. I am especially grateful to God for this opportunity to learn and grow. I am indebted to my thesis advisor, Dr. Charles A. Bleckmann, Ph.D., for his keen logic, timely assistance, and subtle encouragement during this "struggle." I would also like to express my gratitude to my other committee member, Lieutenant Colonel Michael L. Shelley, Ph.D., for his suggestions and thought provoking questions. Special thanks to Dr. Stefan Trapp for providing a copy of the PLANTX model and politely responding to inquiries from this curious student. Lastly, mahalo nui loa to my family and the friends I have made here at AFIT, in particular: Mom, Dad, Zanne, Deb, Carol, Don, Rick, Kris, and Deven for helping me to remain "human" through this endeavor by just simply being there and occasionally providing detours onto the scenic route. Aloha Ahui Ka Kou!

Roy-Alan C. Agustin

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Abstract

This research expands our very limited knowledge on the influence of plants on the fate and effects of TCE (1,1,2-trichloroethylene), providing a screening tool on which to base decisions regarding the need for actual sampling of plants and vegetables, and if necessary, restrictions on the use of TCE-contaminated water. This study assesses the potential for plant uptake of trichloroethylene and derives through simulations the range of values for different combinations of soil organic fraction and soil TCE concentrations which would result in plant concentrations exceeding the TCE maximum contaminant level (MCL) of five micrograms per liter of solution, thereby indicating the type of crops which may be of concern to human health.

First, the physicochemical properties of TCE were screened against relationships reported in published research in order to evaluate the potential for uptake of TCE by plants. The physicochemical properties examined included vapor pressure, Henry's Law constant, water solubility, octanol-water partition coefficient, molecular weight, and half-life. This screening approach indicated that TCE may be transferred to plants via retention by root surfaces, root uptake and translocation, and foliar uptake.

Next, the PLANTX model developed by Trapp, McFarlane, and Mathies was applied to a simplified representation of a soybean plant to determine minimum soil TCE concentrations which would result in plant TCE levels which would exceed the MCL. The simulations revealed that stem and root crops are the most vulnerable to uptake and accumulation of TCE. Significantly higher soil and air TCE concentrations than those observed for the stem and roots are required to produce leaf and fruit TCE levels of concern to human health.

These general procedures were then applied to an existing off-site contamination situation at Hill Air Force Base near Ogden, Utah. The simulations indicate that the

existing concentrations of TCE in irrigation water from contaminated residential wells and springs do not currently result in plant TCE concentrations greater than the MCL.

ANALYSIS OF THE POTENTIAL FOR PLANT UPTAKE OF TRICHLOROETHYLENE AND AN ASSESSMENT OF THE RELATIVE RISK FROM DIFFERENT CROP TYPES

I. Introduction

Problem Background

Air Force Concern. Trichloroethylene (1,1,2-trichloroethylene) (TCE) is viewed as an environmental pollutant that poses risk to human health (USEPA, 1985, 1987, 1992). Leaching of TCE (and other potential toxicants) from waste disposal sites has contaminated water supplies, requiring substantial efforts to remediate TCE-contaminated sites, especially on Air Force bases (Steinberg and DeSesso, 1993:146; Kneeling and Hushon, 1992:49). A resulting corollary concern to direct ingestion of TCE-contaminated water is the consumption of fruits and vegetables irrigated with TCE-contaminated water.

The fate and effects of plant uptake of TCE from contaminated water supplies has become a major concern for at least two Air Force bases. In one case, as a result of a TCE plume originating from Hill Air Force Base (AFB) in Utah, ground water from nearby private wells has been contaminated with 2.3 to 18.5 micrograms of TCE per liter of solution (Radian, 1994:3-35). The well water is currently being used to irrigate fruit trees and home vegetable plots (Radian, 1994:5-5). In the other case, at Reese AFB in Texas, a commercial greenhouse has filed suit against the Air Force, alleging that TCE contamination in its supply of ground water has caused a loss of business (Armstrong Laboratory, 28 October 1993). Preliminary analysis suggests that the greenhouse wells may contain TCE at levels distinctly above the maximum contaminant level (MCL) of 5 micrograms of TCE per liter of solution set by the Safe Drinking Water Act.

Past Researcl. Focus. Unfortunately, little research has been accomplished on the plant uptake of industrial pollutants, such as TCE. Instead, most published literature on plant uptake focuses on agrochemicals, such as pesticides, herbicides, and fertilizers. Nellessen and Fletcher point out that there is essentially no plant-food-chain data available for approximately 75% of the hazardous substances monitored by the EPA (1993:2049). Therefore, an opportunity exists for additional research to investigate the uptake of TCE by plants and vegetables.

Objectives

In order to determine the probability that crops irrigated with water containing TCE could present a health hazard, this research effort will attempt to meet the following objectives:

1. Deduce the potential for plant uptake of TCE based on:
   a. its concentration and physicochemical properties,
   b. site environmental conditions, and
   c. plant characteristics.
2. Using a computerized model of plant uptake processes, derive the minimum TCE soil concentration values for different combinations of soil organic fraction and initial TCE air concentrations which result in TCE plant concentrations exceeding 5 parts-per-billion.
3. Determine the likely locations within plants where TCE may accumulate, thereby indicating the type of crops (e.g., root crops, leafy vegetables, fruits) which may be of concern to human health.

Scope of Research

Previous investigations have provided a procedural framework by which to screen a chemical's relative potential for plant uptake based on its physicochemical properties (Wild and Jones, 1992; Trapp et al., 1990; Ryan, 1988; Topp, 1986; Briggs et al., 1982). The relevant physicochemical properties of TCE will be evaluated against the guidelines provided by these studies. Next, a model will be used to predict the fate of TCE in plants. The model will be applied to a specific and existing situation at Hill AFB in Ogden, Utah. However, no validation with laboratory experiments or field studies will be included in the scope of this thesis. The Hill AFB Environmental Management Directorate has contracted a TCE vegetative uptake study to determine the fate of TCE in plants resulting from the use of TCE-contaminated irrigation water. The contract will commence in early fiscal year 1995 and will consist of experimental research on TCE uptake by carrots, tomatoes, and soybeans (Jines, 1994). The results of the Hill AFB effort could be compared with the conclusions of this thesis.

Possible Benefits

An understanding of the plant uptake and accumulation characteristics of TCE is clearly essential in assessing the exposure pathway of ingestion of TCE-contaminated fruits and vegetables. This research effort will suggest the range of soil-water concentrations at which plant uptake of TCE may pose a significant concern to human health. It will provide a screening tool on which to base decisions regarding the need for actual sampling of plants and vegetables, and if necessary, restrictions on the use of TCE-contaminated water.

Overview

This thesis examines the significance of plant uptake and accumulation of TCE as a human route of exposure. The following chapter reviews the literature necessary to establish the theoretical framework to analyze the mechanisms governing plant uptake of TCE. Chapter three describes in detail the methodology used to achieve the research objectives. Next, chapter four presents findings, data, and analytical results. Finally, chapter five will discuss the significance of findings, draw conclusions, and suggest areas for further research.

II. Literature Review

History of TCE Usage

TCE was first synthesized in 1864 and has been in commercial production for over 80 years (Steinberg and DeSesso, 1993:138). It is a colorless, volatile halogenated hydrocarbon commonly used as an industrial and dry-cleaning solvent, metal degreaser, and fumigant (Windholz et al., 1983:9450). There are no known natural sources of TCE (USEPA, 1985:3-5). Since 1976, the production and use of TCE has been on the decline due to increasing regulation on its use and the increased use of substitute solvents, such as methyl chloroform and methylene chloride (USEPA, 1985:3-5).

Still in 1991, TCE was listed in the United States as one of the "Top 50 chemicals for Largest Releases" with over 35 million pounds of the chemical released to the environment from industrial sources alone (USEPA, 1993:36). TCE releases to different environmental media in 1991 are shown in Table 2.1. In a 1975 United States Environmental Protection Agency (EPA) survey of the water supplies of ten cities, TCE was detected in half the supplies tested at concentrations ranging from 0.1 to 0.5 micrograms of TCE per liter of water (USEPA, 1992:10-1). Although widely distributed in the environment, there is no indication TCE is persistent or that it bioaccumulates in the food chain (USEPA, 1992:10-1).

As a result of its use, accidental spills, leaking storage tanks, and improper disposal practices, TCE is the object of soil and ground water remediation efforts throughout the United States and especially on Air Force installations (Kneeling and Hushon, 1992:49). The major impetus to remediate sites with TCE contamination is the EPA regulation that the MCL for TCE in potable water should not exceed 5 micrograms of TCE per liter of solution (USEPA, 1985, 1987).

Table 2.1 1991 TCE Releases to the Environment. (USEPA, 1993:36) (Pounds)					
Fugitive or Nonpoint Air Emissions	Stack or Point Air Emissions	Underground Injection	Surface Water Discharges	Releases to Land	Total Releases
16,642,065	18,416,403	800	12,750	62,991	35,135,009

Physical and Chemical Properties of TCE

TCE is a colorless, nonflammable liquid with a sweet odor, resembling chloroform. It is "practically insoluble" in water, but highly soluble in lipids (ACGIH, 1986:595; USEPA, 1992:10-1). Reported values of oil/water partition coefficients for TCE range from 900:1 to 960:1 at 37°C, indicating that TCE is highly lipophilic (USEPA, 1985:3-3).

The physicochemical properties of a contaminant influences its environmental fate. Therefore, it is essential that they be understood. Some important physicochemical properties of TCE are shown in Table 2.2.

Table 2.2 Physical Properties of TCE. ([A]USEPA, 1979:52-2; [B]Anderson and Walton, 1992:6)	
Molecular Weight	131.9[B]
Vapor Pressure	60 mm Hg @ 20°C[B]
Henry's Law Constant (dimensionless)	0.397[B]
Boiling Point	87°C[A,B]
Vapor Specific Gravity	4.55 @ boiling point (air = 1)[A]
Solubility in Water	1.1 g/L @ 25°C[A]
Density	1.46 g/ml @ 20°C[A]
Log_{10} Adsorption Coefficient (log K_{oc})	2.6 - 2.7[B]
Log_{10} Octanol-Water Partition Coefficient (log K_{ow})	2.29 - 2.36[A,B]

Health Effects of TCE

The concern over the release of TCE to th . environment arises from its documented toxic effects to mammals. Excessive exposure to TCE results in deleterious effects on a variety of mammalian organ systems, including the central nervous system, liver, and kidneys (ACGIH, 1986:595). However, the extensive literature on the toxicology of TCE is at times conflicting, and substantial arguments exist that TCE is not a human carcinogen (ACGIH, 1986:596; Steinberg and DeSesso, 1993; USEPA, 1992:10-6). The current regulations governing allowable environmental contamination by TCE are based upon studies which demonstrated induction of malignancies in rodents after chronic exposure to very high doses of TCE (Steinberg and DeSesso, 1993:141). The EPA

currently classifies TCE as a probable human carcinogen (USEPA, 1987:3,42). The criterion for this classification is that sufficient evidence from animal studies suggests TCE is a human carcinogen, even though there is inadequate evidence or no data from epidemiological studies to support this conclusion (Cohrssen and Covello, 1989:49).

TCE may be present in plants as a result of direct deposition onto plant surfaces, uptake from the soil, and uptake from the air. Consumption of contaminated fruits and vegetables could be a significant human route of exposure, particularly for farmers and rural and urban residents consuming homegrown fruits and vegetables grown in contaminated soil or irrigated with contaminated water (USEPA, 1989:6-43).

Plant Uptake of Organic Chemicals

Chemicals may enter a plant through at least four main pathways: (1) root uptake and subsequent translocation by the transpiration stream; (2) uptake of vapor from the surrounding air; (3) uptake by external contamination of plant shoots by soil or dust, followed by retention in the plant cuticle or penetration through it; and (4) uptake and transport in oil cells for oil-containing plants, such as carrots, cress, and parsnip (Topp et al., 1986:219). The net chemical uptake by a plant will be the sum of each of these pathways minus metabolic and transpiration losses. Because pathways (3) and (4) are significant only in specific situations or specific plants, they can be discounted as major routes of plant contamination for the general case of plant uptake (Ryan et al., 1988:2307).

Root Uptake of Organic Chemicals. Chemical solutes may enter a plant through its roots along with water and mineral nutrients. The various components of a root tip are depicted in Figure 1. The transport of solution in a plant is through water potential gradients induced by evapotranspiration of water vapor from the foliage to the atmosphere. The chemical solute is absorbed with water from soil solution into the

epidermis which contains the "apparent free space" of the root tissue (McFarlane et al., 1987:847). The "apparent free space" is composed of cellulose and open spaces which allow for water and solute movement between the cortex cells of the root. It accounts for most of the water and solute movement from the soil solution to the endodermis (Lindstrom et al., 1991:130).

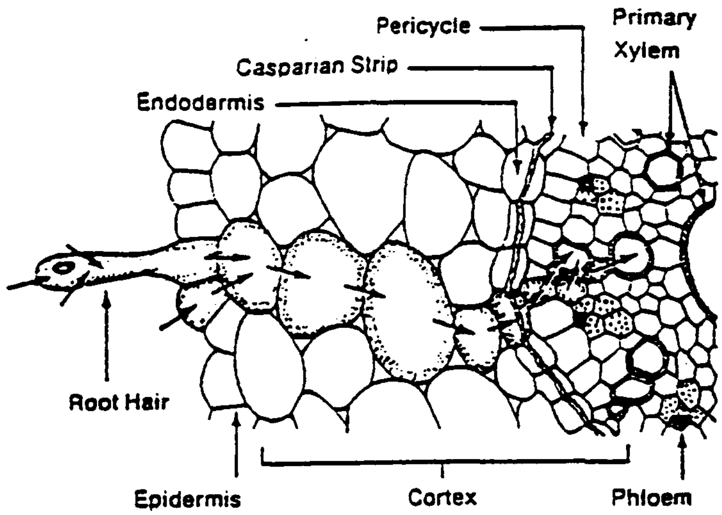

Figure 1. Cross Section of a Generic Plant Root
(Adapted from Hartman et al., 1988:27)

While water passes easily through the membranes of the root, nonpolar (log K_{OW} = 3 to 7) chemicals tend to absorb and become bound to lipids (i.e., fats or fat-like materials) in membranes and the cell walls rather than pass through the epidermis (Bacci et al, 1990:525; Bell, 1992:36). Evidently, nonpolar chemicals are stopped at the root peel level, since the mobility of these chemicals through plant tissues are very low (Bacci and Gaggi, 1985:679; Weber and Mrozek, 1979:415-416). On the other hand, the more polar

the molecule, the more readily it will pass through the outer root membrane. Thus, a selective barrier to chemicals exists at the epidermis.

Chemical solutes which reach the endodermis must pass through the permeable endodermal cell walls and protoplast (that is, living cellular material) before entering the plant's inner tissue. The endodermal cell walls provide surfaces on which chemical compounds may become sorbed, bound, or metabolized (Lindstrom et al., 1991:130). The movement of a chemical solute through the endodermis is dependent on the chemical's polarity and molecular configuration (Paterson et al., 1990:299).

Upon reaching the xylem, the chemical solute is then transported through the plant in the transpiration stream or sap. The xylem serves as the primary vessel for conducting water, dissolved mineral nutrients, and the chemical solute from the roots to all parts of the plant. Chemical movement within the xylem is influenced by bulk water movement controlled by the water potential gradient in the leaves (McFarlane et al., 1987:848).

Foliar Uptake of Organic Chemicals. Air borne pollutants may be transported to and from the surface area of above ground parts of plants in the vapor phase, dissolved in droplets, or in particulate form. Chemicals may enter foliage, fruit, stem, or bark through the cuticle or stomata.

The surfaces of the above ground parts of plants are covered by a non-living, lipophilic membrane--the plant cuticle. The cuticle is imbedded with wax platelets which serve as a barrier to reduce water loss from plants, as well as prevent penetration of environmental pollutants. Stomata are small pores located on leaf surfaces. These pores open and close, allowing carbon dioxide (a material required for photosynthesis) and oxygen (a photosynthesis product) to enter or be released from the plant. Water also enters or escapes through the stomata. Thus, the stomata may act as preferential sites of entry for gaseous pollutants (Bell, 1992:35).

Chemicals contacting leaves may (1) partition into the cuticle from which they may be translocated to other plant parts, or (2) diffuse into the plant through the stomata (Paterson et al., 1990:301). Because the cuticle is composed primarily of wax, it tends to repel water-soluble chemicals while sorbing lipophilic compounds. Lipophilic compounds are chemicals which have an affinity for fats and are generally insoluble in water. Because of these hydrophobic chemicals' high affinities for cuticular lipids, much of the chemical that contacts the cuticle will remain there in "storage" with little tendency to migrate to other areas of the plant (Paterson et al., 1990:301). Even chemicals which successfully permeate through the lipid component of the cuticle into underlying cells and tissues may or may not be translocated.

In the case of hydrophobic volatile compounds such as TCE, uptake of the pollutant will likely be through the foliage rather than the root system of the plant because the mobility of these compounds in the soil and in the plant transport system is fairly low due to their low aqueous solubility and strong sorption to lipophilic plant tissue (Sabljic et al., 1990:1321; Trapp et al., 1990:1250).

Factors Affecting Plant Uptake of Organic Chemicals

The uptake, transport, and accumulation of organic chemicals by plants depend on: (1) the physical and chemical properties of the compound; (2) prevailing environmental conditions; and (3) plant characteristics.

Physicochemical Properties of the Compound. Uptake of most chemicals by plant roots is a passive process in which chemicals move into and throughout a plant with the transpiration stream (Bell, 1992:36). Thus, certain general principles apply and we can assess a compound's potential for plant uptake based on its physicochemical properties.

An analysis of a chemical's physicochemical properties may be used to predict a chemical's potential to adsorb, volatilize, degrade, and leach in soils and to be absorbed,

translocated, and accumulated by plants. The physical and chemical properties particularly indicative of plant uptake potential include the compound's molecular weight, vapor pressure, Henry's Law Constant, water solubility, octanol-water partition coefficient, and half-life.

Vapor Pressure. The vapor pressure of a liquid or solid is the pressure of the gas in equilibrium with the liquid or solid at a given temperature. It represents a compound's tendency to evaporate and is essentially the solubility of an organic solvent in a gas. In general, the higher the vapor pressure, the more likely a chemical will volatilize from the soil solution to air-filled soil pores and/or the ambient air. Thus, foliar uptake may be significant for chemicals with a high vapor pressure.

Henry's Law Constant. Henry's Law describes the volatilization of organic solutes. The extent of partitioning between the solution and the air above is described by the Henry's Law Constant (H_C):

$$\text{Henry's Law Constant } (H_c) = \frac{16.04 \text{ P M}}{\text{T S}}$$

where P = vapor pressure of pure solute in mm/kg,
M = molecular weight of solute
T = absolute temperature, and
S = solubility in water mg/L.

The higher the value for H_C , the more likely a chemical will volatilize than remain dissolved in water. According to Ryan et al., vapor phase plant uptake may be expected to be significant for compounds with H_C greater than 10^{-4} (1988:2315).

Water Solubility. Water solubility provides a measure of a compound's solubility in water and is an indicator of its mobility in a soil-water system. The higher the aqueous solubility, the more likely a compound will be mobile. Compounds with low water solubilities would be expected to readily sorb to soil, making them unavailable for plant

uptake. Research has shown that for many compounds, uptake into plant roots is inversely proportional to water solubility while transfer to shoots is more efficient for compounds of intermediate solubility (Topp et al., 1986; Briggs et al., 1982).

Octanol-Water Partition Coefficient. The octanol-water partition coefficient (K_{OW}) is defined as the ratio of a chemical's concentration in octanol (an organic liquid) to that in water at equilibrium:

$$K_{ow} = \frac{\text{Concentration in octanol}}{\text{Concentration in aqueous phase}}$$

The K_{OW} is a dimensionless quantitative measure of the lipophilicity and hydrophobicity of a compound. A chemical's K_{OW} is related to its solubility in water, with the more water soluble chemicals having a low K_{OW} while the more water insoluble or lipophilic compounds having a high K_{OW}. The logarithm (log) of a compound's K_{OW} can be used to estimate the chemical partitioning between water and organic adsorbents, predicting the environmental fate of the organic compound. In general, the higher the log K_{OW} value, the more likely a compound will be adsorbed than remain in water. Organic compounds that become bound to soil particulates will be less available for transfer to the plant.

Wild and Jones indicate that compounds with a "high" log K_{OW} value greater than 4.0 have a high potential to be retained by root surfaces, similar to the sorption of organic compounds to soils (1992:111). Research by Briggs et al. suggests that root uptake and translocation is greater for compounds of lower K_{OW} (1982). Trapp et al. state that foliar uptake of the chemical will be important for compounds with a high K_{OW} and a high Henry's Law constant (1990:24).

Molecular Weight. Generally, as molecular weight increases, the compound tends to adsorb more readily to soil, and solubility in water decreases (Szecsody, 1981:4). In

addition, researchers have correlated root and foliar uptake of chemicals to molecular weight, relating plant membrane penetration to molecular size (Sablijc et al., 1990; Topp et al., 1986:226). Topp et al. reported a negative correlation between total uptake by barley and a chemical's molecular weight for both volatile and non-volatile compounds (1986:226):

$$\log CF = 5.943 - 2.385 \bullet \log M$$

where CF = barley concentration factor, and
M = molecular weight.

Topp et al. further concluded that molecular weight as a substance property was more suitable for predicting plant uptake of chemicals than the octanol-water partition coefficient (1986:227).

Half-life. Plant uptake of most chemicals is concentration dependent. Many chemicals degrade with time as a result of a number of processes, including chemical transformation as they react with other substances, phase-transfer as a chemical volatilizes, or biological transformation by microorganisms. Chemical concentration in plants may also decrease as a result of dilution by plant mass increase (due to plant growth) and by transpiration loss of the chemical (Topp, 1986:222). Furthermore, chemicals may also be metabolized by plant processes, complicating efforts to estimate plant uptake and accumulation of chemicals (Wild and Jones, 1992:101; McFarlane et al., 1987:852-853). Plant metabolism of anthropogenic substances is discussed in more detail in Chapter 3.

A convenient way to address the complex processes affecting a chemical's persistence in a media is to simply combine the degradation processes into a single overall half-life. The half-life, $T_{1/2}$, describes the time required for the concentration of a

chemical to be decreased by 50 percent. The concentration of a substance is modeled with a simple exponential decay relationship: (Masters, 1991:71)

$$C(t) = C(0)e^{-Kt}$$

where K is a reaction rate coefficient (time^{-1}),
$C(0)$ is the initial chemical concentration, and
$C(t)$ is the concentration at time t.

The half-life, $T_{1/2}$, is related to the rate constant K by the following equation:

$$T_{1/2} = \frac{0.693}{K}$$

Ryan et al. developed a classification system to distinguish between the degradability of compounds, i.e., class A less than 10 days; class B between 10 and 50 days; and class C greater than 50 days (1988:2301). Compounds with longer half-lives will have a more pronounced effect on plant uptake because of the potentially longer time to which a plant is exposed to the chemical. Compounds that are rapidly lost from soil will be less significant for the root uptake and translocation pathway.

Bioconcentration Factors. The movement of xenobiotic chemicals from soil to shoots can be described by a series of consecutive partitions between soil solids and soil water, soil water and root, and then the transpiration stream and plant tissues, including the root, stem, and leaves. Concentration factors are a useful way of describing the relative concentration of an organic chemical in particular plant parts. For example, for low concentrations (i.e., the lower part-per-million range), the root concentration of a chemical is linearly related to its concentration in the medium (Topp et al., 1986:222).

Shone and Wood described uptake of a chemical into roots by a Root Concentration Factor (RCF), which was defined as: (1974:392)

$$RCF = \frac{\text{Concentration in roots (ug/g fresh weight)}}{\text{Concentration in external solution (ug/mL)}}$$

Shone and Wood also described the efficiency of a compound's translocation to shoots after root uptake by the Transpiration Stream Concentration Factor (TSCF). The TSCF was defined as: (Shone and Wood, 1974:392)

$$TSCF = \frac{\text{Concentration in transpiration stream (ug/mL water transpired)}}{\text{Concentration in external solution (ug/mL)}}$$

Briggs et al. expressed the corresponding concentration of the chemical in the plant stem with a Stem Concentration Factor (SCF), defined as: (1983:495)

$$SCF = \frac{\text{Concentration in stem (ug/g fresh weight)}}{\text{Concentration in external solution (ug/mL)}}$$

The partitioning of a chemical within a plant can be related to the octanol-water partition coefficient, such that chemicals with high log K_{OW} values are most likely to be sorbed by the soil and/or plant root. Compounds with lower K_{OW} values are expected to be translocated within the plant, possibly reaching the above ground areas of the plant. Briggs et al. evaluated the uptake by barley of 18 chemicals and correlated these concentration factors to the octanol-water partition coefficients of the chemicals (1982). They found that there was a linear relationship between log K_{OW} and log RCF, where root uptake was greatest for the more lipophilic chemicals. Translocation to shoots was

shown to be most efficient for compounds with intermediate polarity, having values of log K_{OW} between 1.5 and 2.0.

Bacci et al. determined leaf/air bioconcentration factors for a number of organic chemicals and correlated these with K_{OW} and H_C (1990). They found that a high H_C will tend to reduce the bioconcentration potential of highly lipophilic chemicals. Similarly, Reischl et al. also developed leaf/air bioconcentration factors based on vapor pressure and H_C for nine chlorinated hydrocarbons (1989:471). However, the derived leaf/air bioconcentration factors consider only vapor adsorption of organic compounds and does not incorporate the contribution of particle-bound deposition

Environmental Conditions. Soil properties, especially organic content, are determining factors in the fate of chemicals in the plant-soil environment. Temperature, soil moisture, and soil pH are other critical factors affecting plant uptake.

Organic Fraction of the Soil. The organic fraction of soil is composed of microorganisms, a mixture of decomposing plant and animal residues, and their breakdown products. Sorption of volatile chlorinated aliphatic compounds, such as TCE, to soil is attributable primarily to soil organic matter (La Poe, 1985:162; Szecsody, 1981:3). Therefore, the degree of sorption of the non-ionic organic compound, and its availability for plant uptake, is dependent on the organic carbon content of the soil.

Soil Moisture Content. Sorption of organic chemicals is greater in dry soils than in wet soils because surfaces that would normally adsorb water become available to the chemical. Furthermore, Spencer et al., conclusively demonstrated that in the case of relatively nonpolar organic chemicals, vaporization of the chemical was greater in wet soils than from dry soils because of the increased vapor pressure resulting from displacement of the chemical from the soil surface by water (1982:20).

Temperature. Temperature affects a chemical's solubility and vapor pressure, and thus influences its adsorption on to soils and uptake by plants. Generally, an increase in

soil temperature leads to decreased adsorption (Bell, 1992:15). However, temperature effects can also increase the drying rate of the soil surface, thereby decreasing vapor density and resulting in less volatilization of the chemical from the soil surface than at a lower temperature (Spencer et al., 1982:20).

Soil Acidity (pH). The pH or acidity of the plant-soil environment affects a chemical's bonding potential (Bell, 1992:15). La Poe reported that variations in pH over the range normally encountered in soil solution (4 to 9) has negligible influence upon sorption of TCE onto mineral soil (1985:220). At slightly basic conditions, nonionic compounds are moderately adsorbed. However, for highly organic soils, pH may indirectly influence sorption of TCE and other compounds by controlling the solubility of certain soil organic matter constituents, such as lignin and humic acid (La Poe, 1985:252).

Plant Characteristics. A plant's species and variety influences the uptake of organic chemicals. Bell et al. reported in Contaminated Soil '88 that in research conducted by Hermanson and others, plant uptake varied by as much as 400 percent between different carrot varieties grown in endrin (a pesticide) contaminated soil (1988:456). Plant characteristics, such as type of root system, shape and chemical characteristics of the leaves, and lipid content, affect the chemical uptake and distribution within plants (Wild and Jones, 1992:98). Although there has been no systematic examination of plant responses to organic chemicals in soil, it does appear there is variation in uptake both between species and within the same species on an individual level (Ryan et al., 1988:2315). Anderson and Walton demonstrated that in experiments where environmental conditions, such as temperature, soil organic fraction, and soil moisture content were kept constant, plant uptake of TCE appeared to be dependent on plant characteristics and the physicochemical properties of the chemical (1992: 164).

Plant Uptake Model Research

Plant uptake models have been developed using network thermodynamics, fugacity, and mass balance, to describe the transport and accumulation of chemicals in the various compartments of the soil-plant system. This section will present examples of each of these approaches to describe plant uptake and accumulation.

Fugacity-Based Models. Fugacity is the "escaping tendency" of a chemical substance from a phase (Mackay and Paterson, 1981:1007). When the "escaping tendency" from one phase exactly matches that from the other, equilibrium is achieved. In the atmosphere, fugacity is usually equal to the partial pressure of the chemical. At low concentrations, fugacity is linearly related to concentration by a proportionality factor called the fugacity capacity.

Riederer used this equilibrium partitioning approach to assess the atmosphere-to-vegetation transfer in different model leaf compartments of persistent organic chemicals (1990). The model is based on the fact that at equilibrium equal fugacities are established in all compartments of a system regardless of the nature or the physical states of the compartments. Inputting the aqueous solubility, saturation vapor pressure, and K_{OW} of the chemical of concern, Riederer's model estimates air-to-vegetation bioconcentration factors and equilibrium concentrations in leaf tissues. The model also assists in predicting leaf locations where a chemical will preferentially accumulate.

However, the model admittedly assumes chemicals are persistent and are not translocated and/or metabolized within the leaf or diluted by growth. A complete description of plant uptake and accumulation of xenobiotic chemicals should incorporate these two processes and also consider uptake and loss kinetics and chemical concentration dilution due to growth.

Network Thermodynamics Model Simulation. Network thermodynamic theory "combines the principles of irreversible thermodynamics with the conceptual framework

of network theory to describe transport and storage in complex biological structures" (McCoy, 1987:179). McCoy applied network thermodynamics to the simultaneous, coupled transport of water and trace organic solute in a single leaf/single root representation of a soybean seedling under conditions of constant transpiration and passive solute transport (1987). This mechanistic mathematical model of plant transport processes uses coefficients (e.g., hydraulic conductivity of different plant tissues) and equations (e.g., the Kirchoff current and loop laws) to describe the flux of water and trace organic solute between plant compartments. The model distinguishes between convective long-distance transport in the xylem and phloem and the combined convective and diffusive short-distance transport in the apoplast and symplast. McCoy's model provides time dependent estimates of the relative concentration of trace organic solutes in the various compartments of the soil-plant system. The model assumes steady-state conditions with no uptake of water for plant growth and only solute pulse-loading from the soil with no contaminant inputs from the atmosphere.

Mass Balance Approach. Several models based on principles of conservation of mass have been developed (Boersma et al., 1990, Trapp et al., 1994). These models also define a generic plant as a set of adjacent compartments, each representing major plant tissues involved in the transport and accumulation of water and solutes. The formulated system of equations describes chemical mass in each compartment as a function of time.

The PLANTX model developed by Trapp et al. is a particularly versatile model applicable to different plant species and most (nondissociating) organic chemicals (1994). This model integrates the physicochemical properties of the contaminant with the anatomical and physiological processes of plants. Unlike other models which focus on chemical uptake through either the roots or foliage, the PLANTX model considers simultaneous uptake from soil, solution, or atmosphere, and also incorporates the metabolism and accumulation of anthropogenic chemicals in roots, stems, leaves, and

fruits. One drawback of this model is that it does not consider translocation from foliage uptake to the roots. Thus, the concentration of the pollutant in the roots may be slightly low. However, the ease (requires only a few well-known input data) and speed of the PLANTX model make it an ideal tool for describing plant uptake. This model will be used in this thesis to model the uptake and accumulation of TCE and will be described in more detail in the following chapter on Methodology.

III. Methodology

Assumptions

Several assumptions are key to the methodology used in this thesis.

- The uptake of xenobiotic chemicals by plants is a passive process.
- The general plant model assumes initial conditions in which plant parts contain no anthropogenic chemicals.
- The soil and atmospheric compartments exhibit continuous source loading in which their pollutant concentration remains constant throughout the life of the plant.
- The general plant model considers soil, root, stem, leaf, fruit, and atmospheric compartments to be individually homogeneously mixed (Trapp, 1994).
- Because metabolite character cannot yet be predicted, the fate and effects of metabolites will not be considered (Trapp et al., 1994:415).
- Phytotoxic effects of TCE are not considered when assessing the potential for uptake by plants.

Physicochemical Screening of TCE

The potential for plant uptake of TCE will be assessed on the basis of physicochemical parameters of TCE with consideration of significant environmental conditions influencing the bioavailability of TCE. The parameters of TCE pertinent to its bioavailability to and uptake by plants are available from published literature. These properties will be compared with the results of previous research relating physicochemical properties to plant uptake. This initial screening of TCE will also provide an indication of the likely pathway (root uptake and translocation versus foliar uptake and assimilation) for TCE uptake by plants.

TCE Exposure Concentration Derivation

The PLANTX model developed by Trapp and others will be used to estimate the concentrations of TCE in specific plant compartments resulting from specified initial conditions. Different combinations of soil organic fraction and varying initial concentrations of TCE in the soil and air will be tested to derive the range of values which result in a concentration exceeding 5 parts-per-billion TCE per plant wet weight (μg/kg)--approximately equal to the Safe Drinking Water Act MCL of 5 micrograms of TCE per liter of solution--in specific plant parts (i.e., roots, stems, leaves, and fruits). The resulting range of values will provide guidelines by which to base decisions on the need for actual sampling of plants and vegetables at sites with TCE soil contamination or where TCE-contaminated irrigation water is used. Furthermore, the PLANTX simulations will indicate likely locations within plants where TCE may accumulate, and therefore which type of crops (e.g., root crops, leafy vegetables, fruits) are of probable concern.

PLANTX Model Description

Trapp and others developed and validated a conceptual model for the uptake of anthropogenic chemicals into plants (1994). The model describes the dynamic uptake of an organic chemical from soil, solution, or atmosphere, the metabolic transformation rate of the parent compound, and the accumulation of the parent compound and metabolites in individual plant compartments (i.e., root, stem, leaf, and fruit). Figure 2 shows the conceptual organization of the model. A copy of the Fortran 77 code for the model may be found in Appendix A.

Physical, chemical, and physiological processes considered in the model include: (1) organic chemical partitioning between plant tissue and plant sap; (2) diffusive exchange between the soil and roots; (3) uptake and translocation with the transpiration stream;

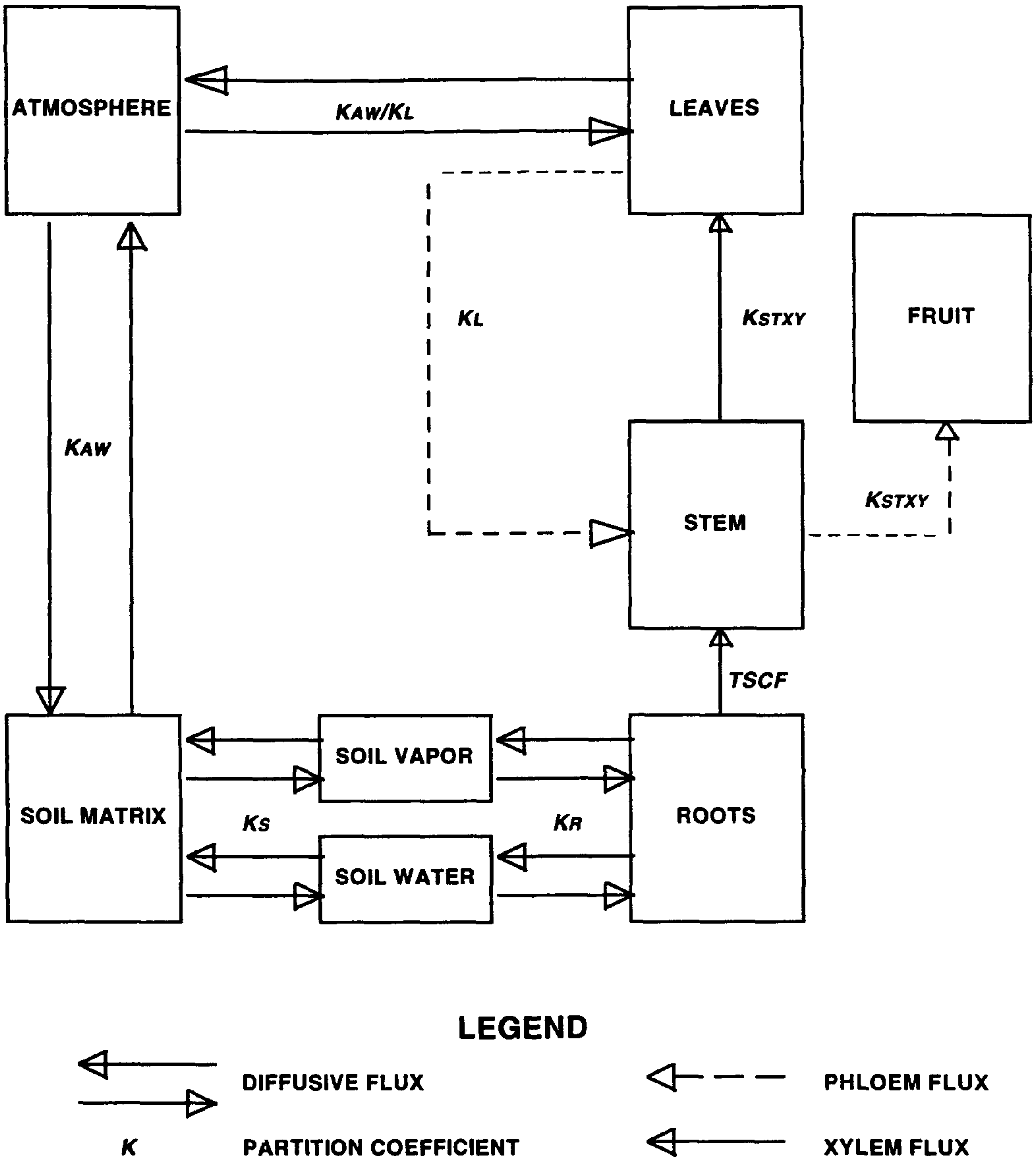

Figure 2. Conceptualization of the PLANTX Model in Terms of Compartments and Transport Pathways (Adapted from Trapp et al., 1994:415)

(4) transport with the assimilation stream into fruits; (5) diffusive exchange between air and leaves; (6) metabolism; and (7) dilution by growth.

Organic Chemical Partitioning with Plant Tissue. Solutes sorb to various materials in the plant, partitioning between water and the lipid and proteins of the cell walls and membranes (Boersma et al., 1988:406; Briggs et al., 1983). Non-ionized chemicals accumulate in the root via two processes: (1) uptake into the aqueous phase in roots contained in the apparent free space and within the root cells, and (2) partitioning of chemicals to lipophilic root solids (Briggs et al., 1982:503). The more lipophilic the chemical (i.e., higher K_{OW}), chemical accumulation in the root will be dominated by the partitioning process rather than aqueous phase uptake. Following uptake by the root, a reversible partitioning process may occur between aboveground plant tissue (i.e., stem, leaves, and fruit) and the xylem and phloem sap (Briggs et al., 1983:500).

The PLANTX program models the partitioning process through a dimensionless sorption coefficient, K_{PW}: (Trapp et al., 1994:414)

$$K_{PW} = CP / CW = (WP + fatP \bullet K_{OW}^{ZP}) \bullet \rho P / \rho W$$

where CP is the equilibrium concentration in the plant tissue (kg/m^3),
CW is the concentration in the surrounding solution (kg/m^3)
WP is the water fraction of the plant tissue (wet weight),
$fatP$ is the lipid fraction of the plant tissue (wet weight),
K_{ow} is the partition coefficient between n-octanol and water,
ZP is an exponent to correct differences between plant tissue lipids and n-octanol [0.77 for roots and stems (Briggs et al., 1982:500); 0.95 for leaves (Briggs et al., 1983:498)],
ρP is the plant tissue density (g/cm^3), and
ρW is the density of water (g/cm^3).

Diffusive Exchange Between Soil and Roots. Movement of water and solutes into a plant occurs by mass flow (advective flow) or diffusion (Boersma et al., 1988:404; Salisbury and Ross, 1969:122). Diffusion is the process by which a solute moves from areas of higher concentration to areas of lower concentration. The PLANTX model accounts for the diffusive exchange occurring in air- and water-filled pores between the soil and roots. Fick's first law of diffusion describes the flux of a solute under steady state conditions: (Fetter, 1988:389)

$$F = -D \bullet dC / dx$$

where F = mass flux of solute per unit area per unit time,
D = diffusion coefficient (area/time),
C = solute concentration (mass/volume), and
dC/dx = concentration gradient (mass/volume/distance).

It applies a solution for Fick's first law of diffusion to a cylindrical surface to solve for the diffusive flux of a chemical to roots in air- and water-filled pores, N_{DR} (kg/s): (Trapp et al., 1994:414)

$$N_{DR} = (K_{AW} \bullet DGeff + DWeff) \bullet (CS / K_S - CR / K_R) \bullet 2 \bullet XL \bullet \pi / [\ln(R2 / R1)]$$

where K_{AW} is the dimensionless Henry's Law Constant (air-water),
DGeff is the effective diffusion coefficient in air-filled pores (m^2/s),
DWeff is the effective diffusion coefficient in water-filled pores (m^2/s),
CS is the concentration in soil (kg/m^3),
K_S is the dimensionless partitioning coefficient between soil and water,
CR is the concentration in the root (kg/m^3),
K_R is the dimensionless root-water partitioning coefficient,
XL is total root length (m),
*R*1 is the root radius (m), and
*R*2 is the radius of a boundary zone surrounding the roots (*R*1 + 0.001m) in which *R*2 - *R*1 is the diffusion length.

Uptake and Transport with the Transpiration Stream. In a plant, water moves upward from roots to stems to leaves primarily through xylem tissue (Salisbury and Ross, 1969:168). The PLANTX model uses a series of partitioning equations to describe the transport of chemical solutes in the xylem with the transpiration stream.

Mass flow of solute with the transpiration stream, N_T (kg/s), depends on the flow of transpiration water:

$$N_T = QW \bullet CW$$

where QW is the flow of transpiration water (m^3/s), and
CW is the external soil solution concentration (kg/m^3) equal to CS/K_S.

Following absorption of the soil-water solution into the cortex or outer tissue of the root, the solution moves to the center of the root where it encounters the endodermis and the water impermeable Casparian strips. Chemicals may become sorbed, bound, or metabolized in the endodermis before reaching the xylem (Paterson et al., 1990:299). Movement through the endodermal pores and entrance into the xylem is dependent on the lipophilicity of the chemical (Trapp et al, 1994:414; Briggs et al., 1983:492). Briggs et al. expressed the fraction of chemical concentration in the external soil-water solution which can be found in the xylem, TSCF, with K_{ow}: (1983:498)

$$\mathrm{TSCF} = 0.784 \bullet \exp[-(\log K_{ow} - 1.78)^2 / 2.44]$$

TSCF describes the efficiency by which a chemical is translocated to shoots from root uptake. The above equation reveals that an optimum lipophilicity for maximum translocation to shoots occurs at a log K_{ow} value of 1.78, resulting in a maximum TSCF

of 0.784. The resulting concentration in the xylem sap CXy (kg/m3) is then:

$$CXy = TSCF \bullet CW$$

The fraction of the chemical that enters the plant and is translocated within the xylem to the stem, N_{TSt} (kg/s) is: (Trapp et al., 1994:414)

$$N_{TSt} = QW \bullet CXy = QW \bullet TSCF \bullet CW$$

The portion of the chemical that enters the plant with the transpiration stream but is reflected by the endodermis, N_{TR} (kg/s), accumulates in the outer portion of the roots: (Trapp et al., 1994:414)

$$N_{TR} = N_T - N_{TSt} = QW \bullet (1 - TSCF) \bullet CW$$

Upon leaving the stem, the concentration in the xylem sap, CXy (kg/m^3), is equilibrated with the stem concentration, CSt (kg/m^3): (Trapp et al., 1994:415)

$$CXy = CSt \,/\, K_{STXY}$$

where K_{STXY} is the partition coefficient between the stem and xylem sap.

The flow of the chemical out of the stem and into the leaf compartment, N_{TL} (kg/s) is given by: (Trapp et al., 1994:415)

$$N_{TL} = QW \bullet CSt \,/\, K_{STXY}$$

This flux out of the stem results in a decrease of chemical concentration in the stem and an increase of chemical concentration in the leaf compartment.

Transport with the Assimilation Stream into Fruits. Materials produced by photosynthesis in the leaves move to other parts of the plant through the phloem tissues (Salisbury and Ross, 1969:168). While the more hydrophobic chemicals tend to sorb to and remain in the waxy cuticle of the leaves, water-soluble pollutants in the leaf compartment may be transported via this assimilation stream with nutrients and other organic matter from the leaves to the stem, roots, and fruit. (Paterson et al., 1990:301).

The only transport in the phloem considered by the PLANTX model is the flux from the leaf to the stem and then into fruits. The phloem sap is assumed to be in equilibrium with the leaf. The mass transfer of the chemical from the leaf to the stem, N_{PSt} (kg/s), is described by the following equation: (Trapp et al., 1994:415)

$$N_{PSt} = QP \bullet CL / K_L$$

where QP is the flow of the assimilation stream (m^3/s),
CL is the concentration in the leaf (kg/m^3), and
K_L is the dimensionless partition coefficient between leaves and water

and is treated as a gain in pollutant mass to the stem and a loss from the leaf.

In the stem, the chemical concentration in the phloem sap is equilibrated with the stem, arriving at the same concentration as that in the xylem sap leaving the stem. The phloem flux of the chemical from stem to fruit, N_{PF} (kg/s), is described by: (Trapp et al., 1994:415)

$$N_{PF} = QP \bullet CSt \, / \, K_{STXY}$$

The phloem flux from stem to fruit results in a loss of pollutant mass from the stem and a gain within the fruit.

Diffusive Exchange between Air and Leaves. Vapor-phase chemicals may diffuse into/from leaf surfaces. The chemical flux between the atmosphere and leaf compartments, N_{La} (kg/s), depends on the resistances of the stomata, *GS*; the cuticle, *GC*; and the unstirred boundary layer adjacent to the leaf surface, *GA*. These resistances or "conductances" are equivalent to mass transfer coefficients (Riederer, 1990:831). The conductance of a given chemical can be estimated from the conductance of water vapor by accounting for the effect of molecular size on the diffusion coefficient. The stomata conductance, *GS*, is given by the following equation: (Trapp, 1994)

$$GS = \frac{1000 \bullet QW}{\gamma - h\gamma} \bullet \sqrt{\frac{18}{XMOLW}}$$

where γ is the vapor density (kg/m3),
18 is the molecular weight of water, and
XMOLW is the molecular weight of the compound.

The cuticle permeance or conductance, *GC*, is derived by the PLANTX model through the following relationship: (Trapp, 1994)

$$GC = \frac{10^{0.704 \bullet \log K_{OW} - 11.2}}{K_{AW}}$$

The boundary layer air resistance, *GA*, is calculated from the following equation by the model: (Trapp, 1994)

$$GA = 5 \bullet 10^{-3} \bullet \sqrt{\frac{300}{XMOLW}}$$

The leaf conductance, GL (m/s), is the sum of the parallel conductances of the stomata and cuticle. The total conductance (m/s), G_{Total}, is given by the following equation which accounts for the serial conductance of the leaf and boundary layer: (Riederer, 1990:832)

$$G_{Total} = \frac{1}{1/GL + 1/GA}$$

A schematic diagram of this network of parallel and serial conductances is shown in Figure 3.

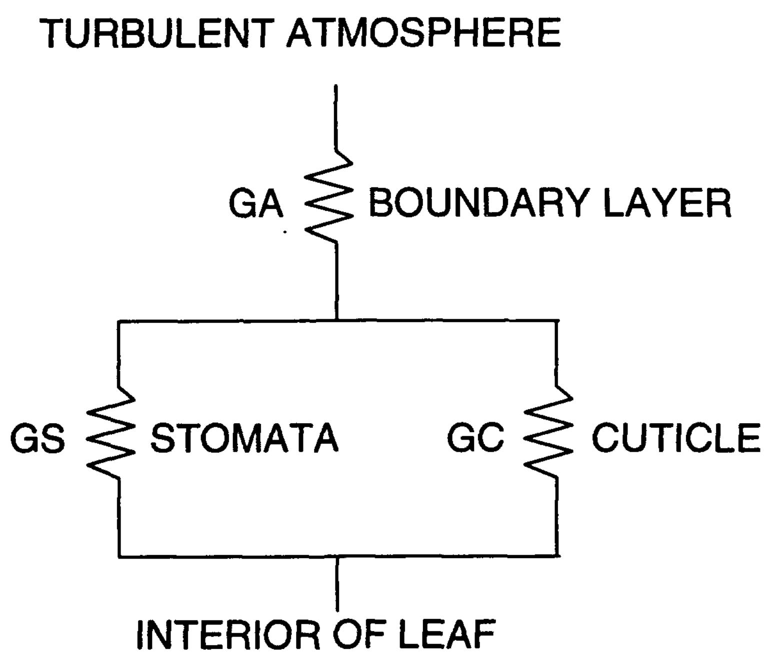

Figure 3. Conductance Network for the Vapor-Phase Transport of Organics Across the Atmosphere/Leaf Interface (Adapted from Riederer, 1990:831)

The total conductance is then used to estimate the vapor-phase chemical transport at the atmosphere/leaf interface. The direction of this reversible flux between leaves and atmosphere depends on the concentration gradient between foliage and air: (Trapp et al., 1994:415)

$$N_{La} = AREA \bullet G_{Total} \bullet (CA - CL \bullet K_{AW} / K_L)$$

where $AREA$ is the leaf area (m^2),
CA is the chemical concentration in the air (kg/m^3), and
CL is the chemical concentration in the leaves (kg/m^3).

Metabolism. Following their uptake, chemicals may be metabolized through biochemical reactions such as oxidation, reduction, conjugation, elimination, and hydrolysis, altering the original molecular structure of the parent compound and producing new substances (Ebing et al., 1984:948). The metabolites formed may be deposited as bound residues in cell walls and other plant tissue, transported, and/or released from the plant (Trapp et al., 1994:415; Wild and Jones, 1992:101-102). Research indicates that plant metabolization of anthropogenic compounds depends on the plant part, plant species, and structure of the anthropogenic substance. Research performed by McFarlane et al. revealed that dinitrobenzene is metabolized in the roots, while dichlorobenzonitrile is degraded only in leaves (1987:852-853). Scheunert et al. found that breakdown of substances and formation of bound residues decreased with increasing level of chlorination and differed between cress plants and barley (1985).

The PLANTX model does not predict the form into which the parent compound will be transformed by physiological processes within the plant. Furthermore, because of the model's inability to predict the chemical characteristics of the metabolites, PLANTX assumes the metabolites to be immobile, remaining in the plant compartment where they are formed. Furthermore, PLANTX assumes the same metabolization rate for all plant

compartments. The model calculates the amount of metabolites formed based on a specified plant metabolization half-life of the parent compound (days), $T_{1/2}$, which is required as input. The first-order reaction rate constant, XR (1/s), is derived from the half-life by the following equation:

$$XR = \frac{\ln 2}{T_{1/2} \bullet 86400}$$

where 86400 is the conversion factor for the number of seconds in a day.

The value for $T_{1/2}$ must be determined outside the model through experimental measurements. Because such experiments could not be performed within the scope of this research effort, a value of 2 days provided by Dr. Trapp served as input for the model simulations (Trapp, 1994).

Dilution Due to Plant Growth. Concentrations of the parent compound and metabolites are diluted by plant growth as the plant mass and volume increases. For simplicity, the PLANTX model assumes dilution by plant growth is linear, following the law of mass conservation in which:

$$C_0 \bullet V_0 = C_t \bullet V_t$$

where C_0 and V_0 are respectively the concentration and volume at time zero, and C_t and V_t are the concentration and volume at time t.

Simulation Input Parameters.

The PLANTX model requires input information on the chemical, plant, and environment for the scenario simulated. A complete set of plant and environmental input

parameters from a 10 April 1992 simulation performed on tetrachlorodibenzo-p-dioxin (TCDD) was received from Dr. Trapp (Trapp, 1994). His plant mass and transpiration rate parameters pertained to a one-hectare plot of soybean plants. The specific parameters were modified for a single soybean plant as explained below. Both the input information received from Dr. Trapp and the input actually used are listed in Tables 3.1 to 3.3.

Plant Input. The model will be applied to a simplified representation of a soybean plant in which the total weight of a specific type of plant part is summed in the specific compartment (i.e., root, stem, leaf, and fruit). The growth of each compartment is characterized by its mass at the start and end of the simulation. The input information provided by Dr. Trapp used initial masses of 1,000 grams for each plant compartment and final masses after a 150-day simulation of 2,500,000 grams for the stem and leaf compartments and 5,000,000 grams for the root and fruit sections.

The plant input data are shown in Table 3.1. The initial masses of the soybean seedlings (i.e., leaves starting to develop at the 11th or 12th node), as well as the lipid and water contents, used in this thesis were adapted from experiments performed by Trapp et al. to validate the PLANTX model (1994:417). The final masses were extrapolated from the nine-day growth of the soybean plants in the experiment to a 100-day simulated growth period. The 100-day growth period corresponds to the soybean growth period in TCDD plant uptake experiments performed by Kew et al. and soil concentration versus half-life simulations performed by Ryan et al. (Kew et al., 1989:1314; Ryan et al., 1988:2302). Conversations with a local commercial soybean grower supported the selected growth period (Carroll, 1991). He expected his crop, which was planted on 31 May 1994, to fully mature by late August. However, the plants would be harvested after the first frost, expected on or about 10 October 1994, to allow the beans to dry.

The leaf area per leaf mass was based on an overall fresh weight density for a soybean leaf of 715 kilograms per cubic meter reported by Riederer (1990:829).

Table 3.1 Soybean Plant Input Parameters		
	Values for a Hectare of Plants from Trapp 1994	Values for Single Plant Used in Simulations
Initial Root Mass (g)	1,000	31.1
Final Root Mass (g)	5,000,000	1298.3
Root Radius (mm)	1.0	1.0
Root Water Content (%)	88.2	94.2
Root Lipid Content (%)	0.6	1.0
Initial Stem Mass (g)	1,000	6.5
Final Stem Mass (g)	2,500,000	135.7
Stem Water Content (%)	75.6	75.6
Stem Lipid Content (%)	1.3	3.0
Initial Leaf Mass (g)	1,000	17.3
Final Leaf Mass (g)	2,500,000	361.1
Leaf Water Content (%)	72.7	72.7
Leaf Lipid Content (%)	1.3	3.0
Leaf Area (cm^2/g)	50	46.62
Initial Fruit Mass (g)	1,000	7.0
Final Fruit Mass (g)	5,000,000	292.2
Fruit Water Content (%)	10	77.0
Growth Period (days)	150	100

Although the RCF, the stem TSCF, and the leaf concentration factor (LCF) could have also been specified, they were instead calculated internally by the program. An example of the input parameter data file for the PLANTX model may be found in Appendix B.

Soil Input Parameters. According to Professor Pete Lane of the Ohio State University Extension, agricultural soils in Southwestern Ohio have organic matter contents ranging from three to five percent (1994). Values of one and five percent were respectively used in the thesis simulations as values for a low- and high-organic fraction soil. These values were considered to be representative of low-organic soils such as Gila Silt Loam (organic matter content = 0.58 %), San Joaquin Sandy Loam (organic matter content = 1.2 %) and Pliocene and Lakeland Association Sands (organic matter content = 1.5-2.0 %); and high-organic matter soil (organic matter content = 5.1) (Spencer et al., 1982:23; Bacci et al., 1985:886; Kew et al., 1989:1316). Uptake of herbicides in a soil with a very high organic matter content of 66.5% was investigated by Harris and Sans in 1967 and reported by Bell (1988:455). This value was also tested. Soil input parameters are listed in Table 3.2.

Table 3.2 Soil Input Parameters

	Values from Trapp 1994	Values Used in Simulations
Organic Carbon Fraction (%)	1.0	1.0, 5.0, and 66.5
Water-filled Pores (vol/vol)	0.30	0.30
Air-filled Pores (vol/vol)	0.10	0.10
Soil Density (g/cm^3)	1.3	1.3

Time Variable Input Data. Soil TCE concentrations were tested to derive a TCE concentration in individual plant parts of five parts-per-billion. An irrigation schedule of every 25 days maintained a constant soil TCE concentration. The Agency for Toxic Substances and Disease Registry (ATSDR) reports mean TCE concentrations of 11 to 30 parts-per-trillion (ppt) in the northern hemisphere (1989:93). An air concentration of 30 ppt was used in the simulations.

Boersma et al. provides a useful estimate of 0.10 milliliters per hour (ml/h) for the transpiration flux from a soybean leaf surface area of 1 cm^2 (1988:411). However, a transpiration rate of 0.00786 ml/h/(cm^2 leaf area) was adapted from the PLANTX model validation experiments (Trapp et al., 1994:417). The transpiration rates were calculated by multiplying this flux value with the mass of the leaf at the specified time and the leaf area per leaf mass of 46.62 cm^2/g. The transpiration rates derived were more than double the 0.003 ml/h/cm^2 used by Dr. Trapp in his TCDD simulation (Trapp, 1994). However, they are based on empirical values which correspond to the plant masses used in this paper's simulations. The time variable transpiration rates assumes the plant experiences linear growth during the 100-day simulation period. The time variable input data are shown in Table 3.3.

Table 3.3 Time Variable Input Parameters

Day	0	25	50	75	100
Soil Concentration (ppm)	Variable	Variable	Variable	Variable	Variable
Air Concentration (ppt)	30	30	30	30	30
Transpiration (ml/h)	6.3	37.8	69.3	100.9	132.4
Humidity (%)	50	50	50	50	50
Temperature (°C)	25	25	25	25	25

TCE Input Data. The molecular weight and log K_{OW} for TCE as listed in EPA documents were used in the simulations (USEPA, 1979:52-2). Per Ryan et al., experimentally derived values for Henry's Law Constants are more reliable (1988:2306). Therefore, the experimentally derived value of 0.397 was used (Anderson and Walton, 1992:6). Finally, Dr. Trapp provided a value of two days for the half-life of TCE within the plant based on the low accumulation of TCE in plants observed by his colleague, Dr. Irene Scheunert (Trapp, 1994). The TCE input data are listed in Table 3.4.

Table 3.4 TCE Input Parameters

Molecular Weight	131.9 g/mole
Log K_{OW}	2.29
Henry's Law Constant	0.397
Half-life Within Plant	2 days

Application to Hill AFB Site

The procedures identified above for the general case of plant uptake of TCE will be applied to a specific situation existing near Hill AFB in Ogden, Utah. Environmental sampling data from investigations conducted in accordance with the Air Force's Installation Restoration Program has been obtained (Radian Corporation, 1994).

Tooele Rail Shop. The Tooele Rail Shop is currently operated by the Tooele Army Depot located on Hill AFB. An open area immediately west of the Rail shop was used for cleaning large train parts. Solvents (including TCE) and petroleum products have

been used at this site. In early 1993, an investigation of ground water conditions along the western perimeter of the base discovered a TCE plume in shallow ground water extending from the Tooele Rail Shop area, located on Hill AFB, off-base to the west. The results of the Air Force's field and laboratory work do not confirm or disprove a connection between low levels of TCE observed at Tooele Rail shop and TCE measured in downgradient off-base wells and springs.

Off-base Field Drains and Wells. Field drains and wells in the Sunset and Clinton areas west of Hill AFB were first installed in the early 1900s (Radian, 1994:3-28). The locations of residential wells and springs, as well as the extent of the TCE contamination at the Tooele Rail Shop and off-base areas, are shown in Figure 4. Field drains were used to control the shallow ground water in the area, making the land suitable for agricultural use. The main use of shallow ground water from the wells and springs is for the irrigation of residential gardens, although the discharge from Martin Spring is used to supply an above-ground swimming pool.

Although TCE has been detected in monitoring wells at levels as high as 5,400 micrograms per liter, concentrations in residential wells and springs range from non-detect to 18.5 micrograms per liter (Radian, 1994:3-35 to 3-47). The TCE concentrations actually observed at the point of use (i.e., the residential wells and springs) will be used to derive plant concentrations using the PLANTX model. The results will indicate whether plant uptake of TCE may be a significant concern in vegetable plots using TCE-contaminated irrigation water at off-base sites near Hill AFB.

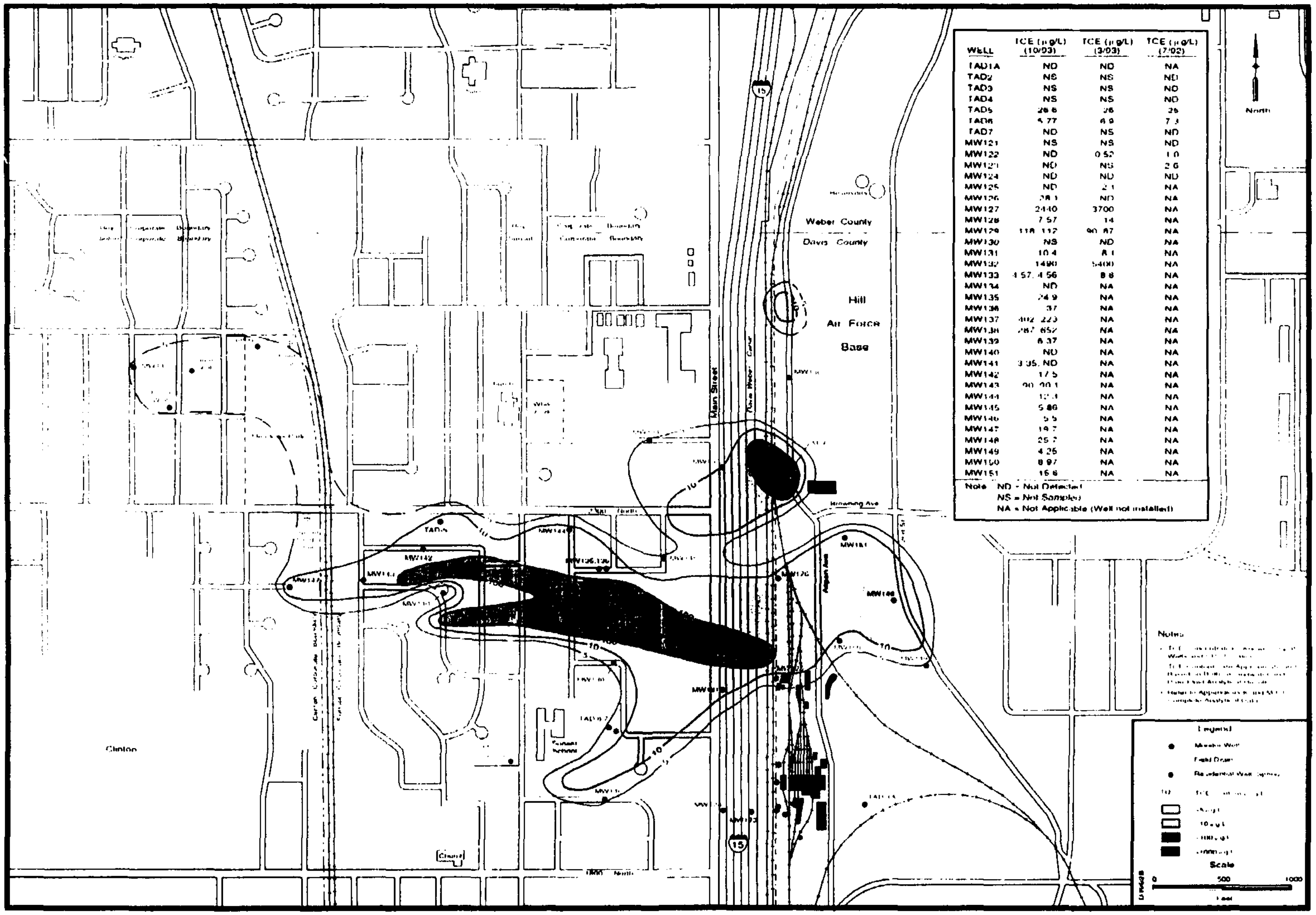

Figure 4 Residential Well and Spring Locations and Areal Extent of TCE Contamination

IV. Results and Discussion

Bioavailability of TCE for Plant Uptake

A comprehensive literature search revealed no work specifically describing the fate of TCE in plant species. Work performed by Anderson and Walton focused on the use of vegetation to enhance in situ bioremediation of TCE (1992). Only one reference each was found respectively pertaining to the plant uptake and accumulation of trichloroethane (TCA) and tetrachloroethene (PCE) which belong to the same group of compounds as TCE--halogenated aliphatics (Bell, 1992; Frank and Frank, 1989). However, considerable research exists identifying relationships between a compound's physicochemical properties and its partitioning and transport into and between various plant parts (Wild and Jones, 1992; Bacci et al., 1990; Paterson et al., 1990; Trapp et al., 1990; Ryan, 1988; Bell, 1988; Travis and Arms, 1988; Topp et al., 1986; Briggs et al., 1982 and 1983; Shone and Wood, 1974). We can exploit these established relationships and the observed behavior of TCA and PCE to understand and assess the corresponding potential for plant uptake and translocation of TCE.

Vapor Pressure and Henry's Law Constant. Topp et al. demonstrated a strong positive correlation between volatilization of chemicals from soil and uptake by barley leaves (1986, 225). Potential volatility of a chemical is directly related to its vapor pressure. TCE's relatively high vapor pressure of 94 mm Hg at 30°C indicates its tendency to volatilize from the soil solution into the vapor phase, enabling uptake into the foliar portions of the plant.

Volatilization of dissolved organic solutes from water is described by Henry's law. Experimentally derived Henry's Law Constants for TCE range from 0.38 to 0.397 (Wild and Jones, 1992:91, Anderson and Walton, 1992:6). These Henry's constants exceed the

10^{-4} value selected by Ryan et al. as the transition point between primary movement in solution and vapor phases (Ryan et al., 1988:2316). Therefore, TCE can be expected to readily partition from the liquid phase to the vapor phase. The resulting vapor phase transport of TCE and its volatilization from the soil compartment into the atmosphere indicates the potential exists for foliar uptake of TCE.

Water Solubility and Octanol-Water Partition Coefficient. As stated earlier in Chapter 2, water solubility is related to K_{OW}, with the more water soluble chemicals having a low K_{OW} and the more insoluble compounds having a high K_{OW}. Furthermore, a compound's adsorption potential to both soil and root surfaces and susceptibility to root uptake and translocation are indicated by its log K_{OW}. Briggs et al. discovered root uptake and translocation approach a maximum for chemicals with a log $K_{OW} = 1.8$ (1982). Wild and Jones noted that chemicals with "high" log K_{OW} (i.e., > 4.0) values are most likely to be sorbed by soil and/or root surfaces (1992:111). Chemicals with "low" log K_{OW} (i.e., < 2.5) values have low adsorption potential and may be translocated within the plant to the above ground parts of the plant. In addition, because it is composed primarily of wax, the cuticle repels water-soluble compounds (Wild and Jones, 1992:100). Therefore, the significance of foliar uptake of water-soluble compounds would be lessened.

Reported log K_{OW} values for TCE range between 2.29 to 2.36 (USEPA 1985:3-1; Anderson and Walton, 1992:6). Furthermore, as a non-aqueous phase liquid, TCE is relatively insoluble in water (ACGIH, 1986:595; USEPA, 1992:10-1). Therefore, TCE would be expected to experience root uptake and subsequent translocation, as well as foliar uptake. However, the residence time of TCE in soil must also be considered since compounds lost rapidly from the soil lessen the significance of uptake through the roots.

Half-life in Soil. Wild and Jones reported a half-life for TCE in sewage sludge of less than one day (1992:85). Focusing on TCE's principal fate process of volatilization, Bell

reported a half-life for TCE in surface soils of four days (Bell, 1992;82). Therefore, following the classification system developed by Ryan et al., TCE would be grouped under Class A--i.e., half-life less than ten days (Ryan et al., 1988). Therefore, because of its relatively short half-life, one would expect TCE to be lost from the soil before being accumulated by the plant through root uptake and translocation. However, periodic irrigation with TCE-contaminated water would replenish the TCE lost through environmental degradation processes, increasing its bioavailability for plant uptake.

Half-life Within the Plant. In addition to the half-life of TCE in the soil system, the degradation of TCE within the plant must also be considered. Although no published documentation on the behavior of TCE in plants was found, according to Dr. Stefan Trapp of the University of Osnabruck, Dr. Irene Scheunert investigated the behavior of TCE in plants, observing its uptake but low accumulation (Trapp, 1994). Dr. Trapp provided a value of two days as input for the PLANTX model, reflecting TCE's rapid metabolization in plants and high volatilization from leaves.

Molecular Weight. Molecular weight has been found to be a reliable indication of plant uptake (Sablijc et al., 1990; Topp et al., 1986:226-227). Given the correlation of molecular weight with a compound's concentration factor (CF) in barley reported by Topp et al., TCE's molecular weight of 131.39 grams per mole results in a CF of 7.76 (1986:226). Therefore, we can expect a total uptake of TCE by barley plants resulting in a plant concentration nearly eight times (based on fresh weight) the TCE soil concentration (based on air-dry weight). Therefore, we conclude that based on molecular weight, plant uptake of TCE is possible.

Summary. Based on its physicochemical properties, the potential exists for TCE to be taken up by plants through both roots and foliage. However, the bioavailability of TCE to plants is strongly influenced by environmental conditions, particularly organic matter content of the soil, as demonstrated by the subsequent PLANTX model simulations.

Derivation of Plant Part TCE Concentrations

Numerous simulations were run using the PLANTX plant uptake model to determine the plant part TCE concentrations resulting from a given set of environmental and plant parameters, but most importantly from a specified soil TCE concentration. A summary of the results for the low- and high-organic fraction scenarios and the actual simulation output files for key simulation runs are incorporated in Appendix C.

Minimum Soil TCE Concentrations Resulting in MCL Plant Part Concentrations. The minimum soil TCE concentrations which result in the TCE MCL of 5 ppb within each plant part are presented in Table 4.1. The residual levels of TCE within the plant resulting from a soil TCE concentration equal to the MCL are also listed. The results indicate that stem crops, such as celery, and root crops, such as potatoes and onions, are the most vulnerable to uptake of TCE.

The general pattern of uptake simulated by the PLANTX model is depicted in Figure 5, which plots the simulation for a specified soil TCE concentration of 6 ppb. The results coincide with the findings of Briggs et al. who reported constant maximum concentrations in barley roots and stems were rapidly attained (within 24 to 48 hours) for chemicals of log $K_{OW} < 3$ (1983:500; 1982:499). These equilibrium concentrations occur when the influx equals efflux at the interface between the plant and soil compartments and between the leaf and atmosphere compartments. Once the equilibrium concentration is reached in both the root and the leaves, an upper limit occurs on the concentration of the chemical in all plant compartments. The TCE concentration in the fruit compartment initially increases but steadily decreases as the metabolization rate begins to surpass the infusion of the parent compound from the stem via the phloem.

Table 4.1 Summary of Significant Soil and Corresponding Plant TCE Concentrations ($\mu g/L$)

SOIL	ROOT	STEM	LEAF	FRUIT
Organic Matter Content = 1.0 %; TCE Air Concentration = 30 ppt				
5	4	4	< 1	< 1
6	4	5	< 1	< 1
7	5	6	< 1	< 1
242	173	192	< 1	5
43,034	30,760	34,180	5	887
Organic Matter Content = 5.0 %; TCE Air Concentration = 30 ppt				
5	1	1	< 1	< 1
27	4	5	< 1	< 1
30	5	5	< 1	< 1
1,057	173	192	< 1	5
187,710	30,760	34,180	5	887
Organic Matter Content = 66.5 %; TCE Air Concentration = 30 ppt				
50	1	1	< 1	< 1

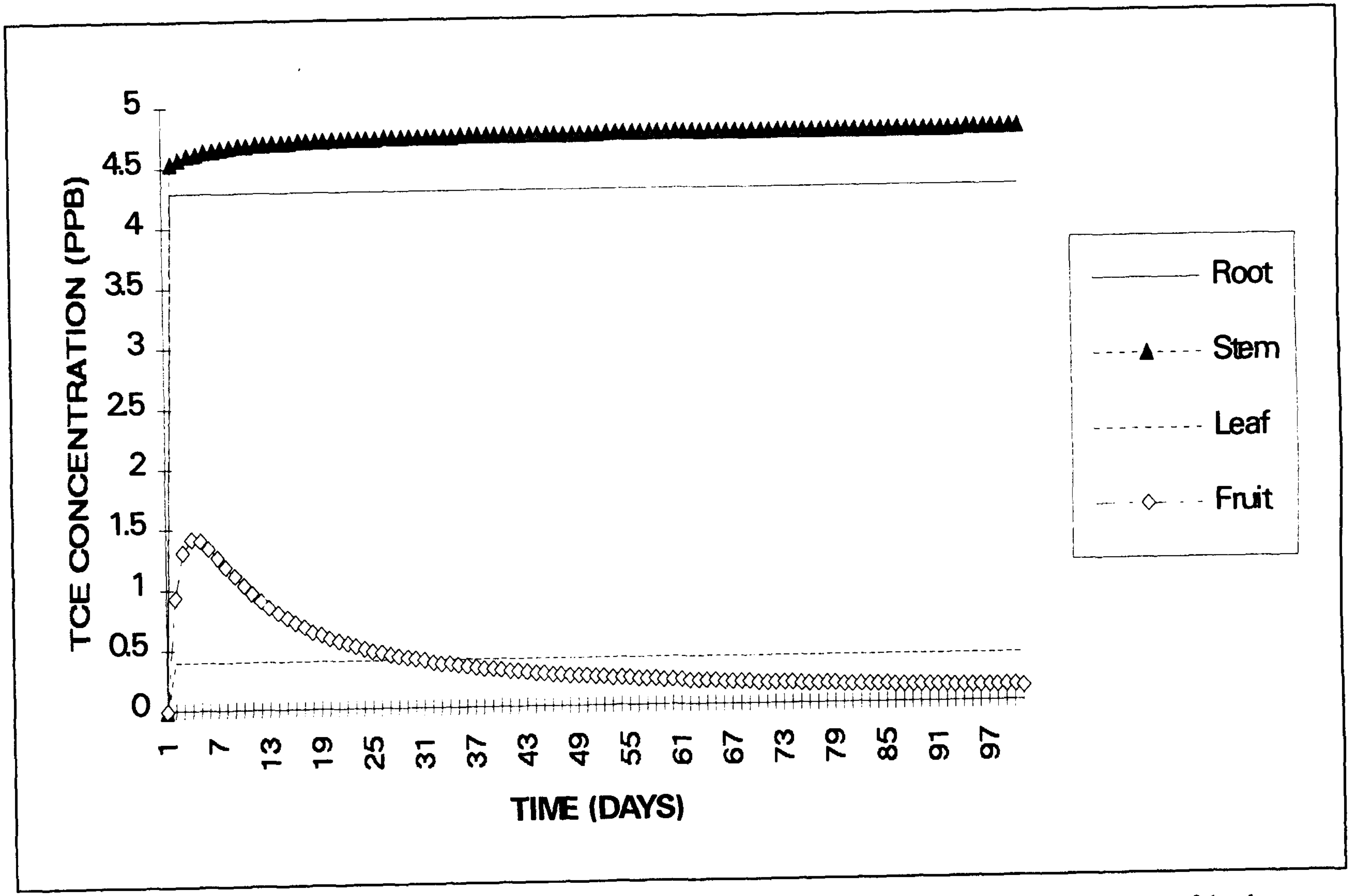

Figure 5. Simulated Soybean Plant Concentrations from Chronic Exposure to a Soil TCE Concentration of 6 ppb.

Figure 6 illustrates the importance of considering the amount of TCE actually taken up by the plant, and not simply the surrounding soil concentration. The chart shows the TCE soil concentrations corresponding to the MCL in the soybean root, stem, and fruit compartments. For both the low and high organic soils tested, the soil concentration must be increased over 35 times to achieve the MCL in soybean fruit (i.e., the seeds) versus the stem and root. This difference is even more pronounced for the leaf compartment. Because significantly higher TCE concentrations are required to achieve the MCL in the fruit compartment, this phenomena is especially fortuitous in the case of soybeans where the seeds are the most economically important part of the soybean. The simulation results coincide with the conclusions of Leroy and Nash who found that the soybean fruit consistently contained the lowest concentration of residues of the organochlorine insecticides they tested (1971:464).

In addition, the simulations confirm the important consequence of changes in environmental conditions, specifically the organic matter fraction and ambient air TCE concentration. Notably higher soil TCE concentrations are required to achieve the MCL in soybean plant parts when increasing the organic matter content from one to five percent. For an organic matter content of 66.5 percent, plant TCE concentrations did not exceed one ppb even for a soil concentration of 50 ppb. The simulations demonstrate the reduction in bioavailability of TCE to the plant as pollutant adsorption to the soil organic matter fraction increases. Agricultural soils with their relatively high organic matter contents (three to eight percent in Southwestern Ohio) would require TCE levels significantly higher than those observed in the simulation runs for an organic matter content of one percent to produce plant TCE concentrations approaching the MCL.

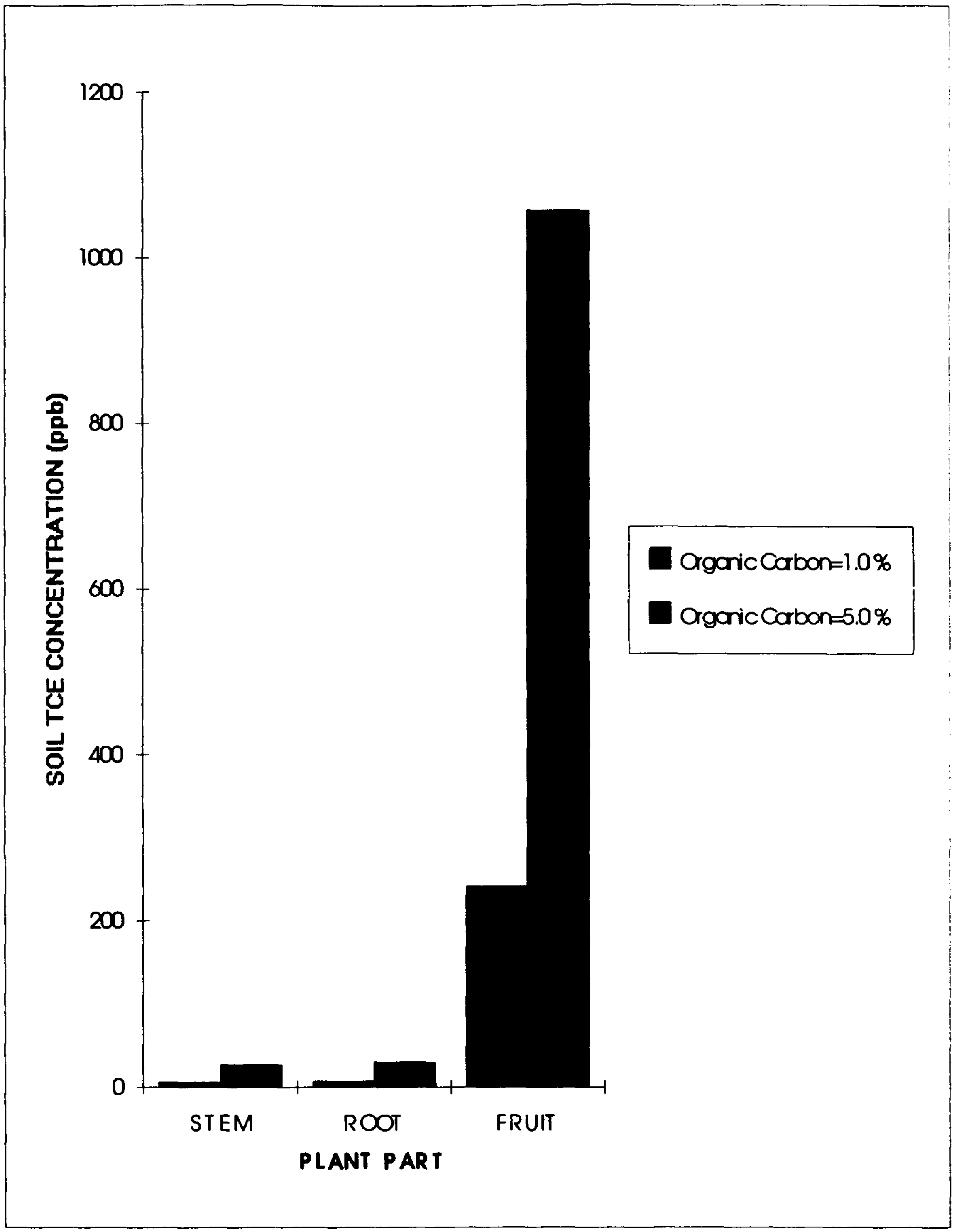

Figure 6. Soil TCE Concentrations Resulting in a Plant Part TCE Concentration of 5 ppb.

Table 4.2 compares plant part TCE concentrations for different ambient air TCE concentrations. For the mean ambient air TCE concentration of 460 ppt in urban/suburban areas compiled by Brodzinsky and Singh as reported by ATSDR, the simulations produced a soybean leaf TCE concentration which exceeded both the soil concentration and MCL for TCE. The soybean root and stem concentrations remained relatively constant despite varying TCE air concentrations for the same TCE soil concentrations. These results demonstrate the importance of foliar uptake and accumulation of volatile organic compounds, such as TCE, in leaves. It is also important to note that the PLANTX model does not consider phloem transport from the leaves to the root. Therefore, the concentration of TCE in the root may be slightly underestimated.

Table 4.2 Soil and Plant Part TCE Concentrations for Different TCE Air Concentrations (μg/L)

SOIL	ROOT	STEM	LEAF	FRUIT
Organic Matter Content = 1.0 %; TCE Air Concentration = 0 ppt				
5	3.574	3.971	< 0.001	0.103
Organic Matter Content = 1.0 %; TCE Air Concentration = 30 ppt				
0	0	< 0.001	0.395	< 0.001
5	3.574	3.971	0.395	0.103
Organic Matter Content = 1.0 %; TCE Air Concentration = 460 ppt				
0	0	< 0.001	**6.049**	< 0.001
5	3.574	3.977	**6.050**	0.103

Plant TCE Concentrations in Residential Areas Adjacent to Hill AFB.

The PLANTX model produced no soybean plant TCE concentrations in excess of the MCL for the highest levels of TCE observed in each of the sampled residential wells and springs located near Hill AFB. The organic matter content of five percent used in the simulation runs is representative of agricultural soils (Lane, 1994). The soil used in vegetable plots would be expected to have comparable organic matter contents. Therefore, use for crop irrigation of water contaminated at the levels of TCE detected in the residential wells and springs do not currently present a health hazard based on the MCL of five micrograms per liter.

Table 4.3 Summary of Maximum TCE Concentrations in Residential Wells and Springs with Resulting Plant Concentrations (µg/L)

LOCATION	SOIL	ROOT	STEM	LEAF	FRUIT
Meadow Park Spring	**18.5**	3.0	3.4	0.4	< 0.1
Omer Well	**11.5**	1.9	2.1	0.4	< 0.1
Sunset Drain	**6.3**	1.0	1.1	0.4	< 0.1
Martin Spring	**6.2**	1.0	1.1	0.4	< 0.1
Meadow Park Drain	2.8	0.5	0.5	0.4	< 0.1
Chicado Well	2.3	0.4	0.4	0.4	< 0.1

However, if in the future the nature and extent of the underlying TCE ground water plume changes and increases the TCE concentration in the residential wells and springs above 27 ppb (which according to the PLANTX model would result in a TCE stem concentration equal to the MCL) or up to the worst case of 5,400 ppb (the highest concentration of TCE observed in area ground water monitoring wells), restrictions on the type of crops irrigated with TCE-contaminated water and grown for human consumption may have to be imposed. However, based on the highest TCE concentration of 5,400 ppb, leaf crops, such as spinach, would still apparently be safe for human consumption, even under the worst case, since a concentration nearly 35 times greater is required to produce a leaf concentration in excess of the MCL.

Conclusion.

Principle Findings and Conclusions

The objectives of this study were to determine the potential for plant uptake of TCE and derive the range of values for different combinations of soil organic fraction and soil TCE concentrations which would result in plant concentrations exceeding the TCE MCL of five micrograms per liter, thereby indicating the type of crops which may present greater relative risk to human health. The procedures outlined above were then applied to an existing TCE contaminant situation existing near Hill AFB, Utah.

Potential for Plant Uptake of TCE. Established relationships between physicochemical properties of chemical compounds and plant uptake reported in previous research support the conclusion that the potential exists for uptake through the root and subsequent translocation of TCE with the transpiration stream. Furthermore, the volatility and relative insolubility in water of TCE contribute to its equally significant uptake through the foliar system of the plant. However, the bioavailability of TCE to plants is strongly affected by environmental conditions in which the plant grows, in particular the soil's organic matter content. Soils with higher organic fractions will tend to adsorb more of the pollutant, reducing the amount of TCE available to be taken in by the plant.

Minimum Soil TCE Levels Resulting in MCL Plant Part Concentrations. The minimum soil TCE concentrations for both the low- and high-organic fraction scenarios which result in the TCE MCL of five micrograms per liter are reshown in Table 5.1. The residual levels of TCE within the soybean plant resulting from a soil TCE concentration equal to the MCL are also listed. The soybean plant simulation results indicate stem and root crops are the most vulnerable to uptake and accumulation of TCE. Significantly

higher soil and air TCE concentrations than those observed for the stem and roots are required to produce leaf and fruit TCE levels of concern to human health.

Table 5.1 Summary of Minimum Soil TCE Levels Resulting in Plant Concentrations Exceeding the MCL (μg/L)

SOIL	ROOT	STEM	LEAF	FRUIT
Organic Matter Content = 1.0 %; TCE Air Concentration = 30 ppt				
5	4	4	< 1	< 1
6	4	5	< 1	< 1
7	5	6	< 1	< 1
242	173	192	< 1	5
43,034	30,760	34,180	5	887
Organic Matter Content = 5.0 %; TCE Air Concentration = 30 ppt				
5	1	1	< 1	< 1
27	4	5	< 1	< 1
30	5	5	< 1	< 1
1,057	173	192	< 1	5
187,710	30,760	34,180	5	887

Hill AFB Scenario. Existing concentrations of TCE in irrigation water from contaminated residential wells and springs do not currently result in plant TCE concentrations greater than the drinking water MCL. Furthermore, agricultural soils with organic matter contents higher than five percent would tend to alleviate the effects of TCE levels even higher than those presently observed in the wells and springs.

Recommendations for Further Research

The findings of this thesis provide only a starting point in assessing the exposure pathway of ingestion of TCE-contaminated fruits and vegetables. Accurate, quantitative experiments are needed to verify the levels of TCE in parts of various plant species resulting from specified soil TCE concentrations and environmental conditions. Potential areas of further research are discussed below.

Phloem Transport to the Root. The PLANTX model only considers movement of chemicals in the phloem between the leaves, stem, and fruit. The phloem (i.e., the conductive portion of the symplast) is primarily responsible for transport of sugars, hormones, and other metabolic solutes to growing and storage plant tissues (Boersma et al., 1988:404). To more accurately reflect the movement of water within the plant, the PLANTX model could be expanded to also consider the transport of the pollutant through the phloem from the leaf to the stem; from the stem to the root and fruit; and from the root back to the stem; and eventually back to the leaf.

Metabolite Fate and Effects. Chemicals may be metabolized by the enzymes and other reactants within the plant (Boersma et al., 1988:403). As stated in Chapter 3, the PLANTX model calculates the amount of metabolites formed based on a specified plant metabolization half-life, $T_{1/2}$, of the parent compound. Although the PLANTX model does not predict the form into which the parent compound is transformed, the model still provides useful insight on the quantity of parent compound transformed within the plant.

Table 5.1 presents a comparison of the mass of the parent compound remaining and the fraction metabolized.

The amount of parent compound transformed is at least an order of magnitude (17 to 33 times) greater than the amount of parent compound remaining. For humans, the nature of the metabolites produced may be of more critical concern than the low concentrations of TCE contained within the plants.

TCE is metabolized by humans primarily in the liver. The first stable metabolite, and the dominant product in humans, is chloral hydrate (Steinberg and DeSesso, 1993:138). Choral hydrate is then further metabolized to trichloroethanol and trichloroacetic acid. For humans, trichloroacetic acid is the major toxic metabolite of TCE (Steinberg and DeSesso, 1993:140). If plant physiological processes produce similar metabolites, the concentration of these metabolites, especially that of trichloroacetic acid, may be more critical to human health than that of TCE. If the concentrations of toxic metabolites present hazards to human health, the limits of allowable soil TCE contamination (based on a plant concentration less than the MCL of five micrograms per liter) presented in this thesis would have to be lowered. As previously stated, the literature search revealed no work specifically describing the fate of TCE and its metabolites, and industrial pollutants in general, in plant species. This scarcity of information emphasizes the need for experimental research addressing the influence of plants on industrial pollutants.

Plant Species and Varietal Differences. The availability of specific plant parameters needed for input into the PLANTX model, limited the application of the model to a simplified representation of a soybean plant. These simulation results were then used to draw general conclusions about relative risk of different crop types based on soybean plant TCE levels resulting from specified soil TCE-concentrations and soil organic matter fraction. However, researchers have found variation in uptake both between species and

Table 5.2 Comparison of Plant TCE and Metabolite Mass

[for Organic Fraction = 1.0% and TCE Air Concentration = 30 ppt]

(μg)

	ROOT	**STEM**	**LEAF**	**FRUIT**
Soil TCE Concentration = 5 μg/L				
TCE	4.64	0.54	0.14	0.03
METABOLITES	82.35	9.76	2.60	1.01
Soil TCE Concentration = 6 μg/L				
TCE	5.57	0.65	0.14	0.04
METABOLITES	98.82	11.71	2.60	1.21
Soil TCE Concentration = 7 μg/L				
TCE	6.50	0.75	0.14	0.04
METABOLITES	115.30	13.66	2.60	1.41
Soil TCE Concentration = 242 μg/L				
TCE	225	26	< 1	1
METABOLITES	3,986	472	28	49
Soil TCE Concentration = 43,034 μg/L				
TCE	39,930	4,638	2	259
METABOLITES	708,700	83,980	33	8,658

within the same species between individual plants (Bell et al., 1988:455). Uptake of endrin between different varieties of carrots were found to vary by as much as 400-percent (Bell et al., 1988:456). Thus, differences in TCE uptake response between plant

species and varieties could result in significantly lower or higher plant TCE levels than those predicted for the soybean plant by the PLANTX model. Further research could obtain, either through experiments or from existing research work, the required plant input parameters for species representative of other crop types (e.g., potatoes for root crops, celery for stem crops, and spinach for leafy vegetables). The additional simulations would present a more comprehensive picture of the relative risk of plant uptake of TCE in different crop types.

Food Processing. The PLANTX model assumes the entire plant compartment to be homogeneously mixed. However, researchers have determined that xenobiotic chemicals are concentrated in certain areas of the plant (Bacci et al., 1990:526). For example, non-polar chemicals in the soil-plant system mostly stop at the root peel level, while in the atmosphere-plant system compounds tend to concentrate in the cuticle. Therefore, although the PLANTX model predicts a root TCE concentration surpassing the MCL of 5 ppb, simply peeling the root prior to consumption may reduce the actual TCE concentration in the root consumed to levels that are no longer hazardous to human health. Moreover, further processing (e.g., cooking) of the vegetables or fruits prior to consumption would probably result in release and vaporization of TCE from plant matter, decreasing the exposure concentration to humans. Understanding food processing's impact on the fate and effects of TCE and its metabolites may present a more accurate picture of the actual exposure concentration received by humans through consumption of contaminated vegetables and fruits.

Phytotoxicity. Organic chemicals may accelerate or reduce plant growth, prevent fruition, or even kill the plant. Information on the response of plants to TCE was not found. The soil TCE concentrations required to achieve a concentration of five-ppb in different plant parts could possibly kill the plant prior to producing a mature crop for harvest, thereby negating the risk of human consumption of contaminated vegetables.

Experimental studies on the effects of different concentrations of TCE on various plant species would present a more realistic assessment of TCE's influence on plants and its effects on the plant levels of TCE resulting from a specified soil concentration.

Epilogue

The public is becoming increasingly aware and involved in environmental issues. The fate and effects of plant uptake of TCE from contaminated water supplies has become a significant concern for at least two Air Force bases. When the public raises the question whether or not TCE contamination of ground water or surface water supplies restricts the use of that water, we as environmental managers should have a competent answer to their concerns. Although the problem requires an even more intensive look than that taken here, this research effort provides that first step towards providing a response to the public's concerns.

Appendix A. PLANTX Model Fortran 77 Code

The following is the Fortran 77 code for the model used in the research. The PLANTX model received from Dr. Stephan Trapp of the University of Osnabruck was slightly modified to correct minor typographical errors, including incorporation of more precise values for pi.

```
C       Program PLANTX
C
C  Stefan Trapp, 08/08/91; GSF-PUC; D-8042 Neuherberg; Germany
C
C ***********************************************************
C  This is a version of the PlantX model with many comments
C
C  Equations: see Theses
C  Dedicated to C. Mc Farlane
C
C *******************************************
C What the model is doing (short description) :
C
C The model simulates the time dynamic uptake of xenobiotic organic
C chemicals into plants.
C There are diffusive exchanges and mass flows
C
C  Diffusive exchanges: between roots and soil solution
C                       between leaves and air
C
C  Mass flows:  Soil solution to roots; into the transpiration stream
C               transpiration stream into the stem; then intop leaves;
C          assimilation stream from leaves into stem; then into fruit;
C
C  Metabolisation: 1st order metabolisation; 1 rate for all plant parts
C
C *** INPUT PARAMETERS: ********
C
C Chemical: molecular weight; logKow; dimensionless Henry's law const.
C and the half life in plants (days).
C
C Plants:
C
C Root: Mass begin, end (g); Radius (mm), Water ,lipid (%),RCF (0=calc)
C Stem: Mass begin, end (g); Water,lipid (%),TSCF (0=calc)
C Leaf: Mass begin end (g) Water,lipid (%),LCF (0=calc)
C Fruit: Mass Begin, Mass End (g), Water content(%); Leaf Area cm2/g
C Soil (solution) OC water pores, air pores (vol/vol) density (g/cm3)
C Numeric: daylength (h), Time step (d), Intervals (#)
C  and then variable for every time needed:
C tnew  Csoil  Cair   tstd  tstn  humid  temp
C tnew  Csoil  Cair   tstd  tstn  humid  temp
C and so on.
C The last tnew is at the same time the end of the simulation
C
C  OUTPUT:  here of parent compound only
C           two files : Plot  (here: parent compound only)
C           results:   Mass balance and some calculated parameters
C
C***********************************************************
C
             implicit real*8 (a-h,o-z)
             real*8 KS,KR,KAW,KL,KSTXY,Kow,Koc,LCF
             character*50 text
              IIN=5
C  IIN: Reads Chemical input
              IDAT=9
C  IDAT: reads Plant and Concentration Scenario from the file Plant.dat
              IOUT=6
C  IOUT writes 'RESULT' to the screen
```

```
                 IOUT1=10
C  IOUT1 writes to the file 'RESULT' (Mass balance, equilibria etc.)
                 IPOUT=7
C  IPOUT writes the time and the concentrations of the plant organs
C        to the file PLOT which is a input to graphic programs
C
                 OPEN(IOUT1,file='result')
                 OPEN(IPOUT,file='plot')
                 OPEN(IDAT,file='plant.dat')
C
C***********************************
C  The following indices are used and describe the variables :
C  S=Soil Water
C  R=root
C  A=air
C  L=leave
C  St =stem
C  F=Fruit
C
C***********************************
C  Definition of input parameters: all internal units are SI (m kg s)
C   whereas the unit of the input is common units
C
C  READ CHEMICAL PARAMETERS interactive
C
       write(iout,*)' Model PlantX  by Stefan Trapp '
       write(iout1,*)' Model PlantX by Stefan Trapp '
       write(iout,*)
       write(iout,*)' Scenario in Plant.dat      '
C
       WRITE(iout,*)'    Title ? (50 Characters) '
C
       read(iin,'(a)') text
       write(iout1,'(a)') text
C
C
       Write(iout,*)'  Molecular weight of the substance g/mol ? '
       read(iin,*) XMOLW
       Write(iout,*)' logKow of that Substance ? '
       read(iin,*) PKow
C
       Write(iout,*)' dim.less Henrys Law Const. of that Substance ? '
       read(iin,*) Henry
C
       Write(iout,*)' Metabolisation Halflife of that Substance (d) ? '
       read(iin,*) T12
C
       write(iout1,101)XMOLW,PKOW,Henry,T12
 101   FORMAT('  MW: ',e11.4,' logKow: ',e11.4,' Henry: ',e11.4,
     &' Halftime: ',e11.4)
C
C  T12 is half life in days; XR is rate in 1/s;
       XRR=0.69315/(T12*86400.)
       XRL=0.69315/(T12*86400.)
       XRSt=0.69315/(T12*86400.)
       XRF=0.69315/(T12*86400.)
C
       Kow=10.**PKow
C  KOC is the sorption to organic carbon; here: following SCHWARZENBACH
C  and WESTALL 1981
```

```
      PKoc=0.72*PKow+0.49
      Koc=10.**PKoc
C
C****************************************
C  Time step optimization part 1:
      it=1
 100  Continue
C
C** Set Loop elements tc zero ************
              CS=0.0
              CR=0.0
              CL=0.0
              CST=0.0
              CF=0.0
              AR=0.0
              AL=0.0
              AST=0.0
              AF=0.0
              SumQW=0.0
              SumTSR=0.0
              Sumdiff=0.0
              Sumdiffa=0.0
              Sumstem=0.0
              SumQP=0.0
              SumTL=0.0
              SumVol= 0.0
              QWtot=0.0
              QPtot=0.0
              th=0.0
              tneu=0.0
              talt=0.0
C
C*** Read plant data from file Plant.dat ************************
C
C   Comment line
      read(idat,*)
C  Root properties:    **********
      read(idat,*)
      read(idat,*)VaR,VeR,R1,WR,fatR,RCF
C     VaR=Root mass in g begin, VeR = end, R1 = Root Radius (mm),
C     WR = Water content (%), fatR = lipid content (%)
C  conversion to SI units
      VaR=VaR*1.D-6
      VeR=VeR*1.D-6
      R1=R1*1.D-3
      R2=R1+0.001
      WR=WR/100.
      fatR=fatR/100.
C  Stem properties:    *************
      read(idat,*)
      read(idat,*)VaSt,VeSt,WSt,fatSt,TSCF
C     VaSt=Stem mass in g begin, VeSt = end,
C     WSt = Water content (%), fatSt = lipid content (%)
C  conversion to SI units
      VaSt=VaSt*1.D-6
      VeSt=VeSt*1.D-6
      WSt=WSt/100.
      fatSt=fatSt/100.
C
C  Leave Properties:  ******************************
```

```
         read(idat,*)
         read(idat,*)VaL,VeL,WL,fatL,LCF
C    VaL and VeL: Mass begin and end (g);
C    WL and fatL: Water and lipid content (%); LCF = Leaf conc. factor
         VaL=VaL*1.D-6
         VeL=VeL*1.D-6
         WL=WL/100.
         fatL=fatL/100.
C    Fruit Properties and Area leaf cm2/g **********
         read(idat,*)
         read(idat,*)VaF,VeF,WF,XMA
C   Area is cm2 leaf per g weight of the leaf.
         VaF=VaF*1.D-6
         VeF=VeF*1.D-6
         WF=WF/100.
C   initial volumes
         VR=VaR
         VL=VaL
         VST=VaSt
         VF=VaF
C   Soil:   ********************************************
         read(idat,*)
         read(idat,*) orgC, PW, PA , Roh
C   orgC is organic carbon content (vol/vol), PW and PA are pores in
C        water and air (vol/vol), Roh = density (g/cm3)
C
C   Read Numeric and time parameters    ****
                 read(idat,*)
                 read(idat,*) tday,Tend,dt,Nint
                 read(idat,*)
C   Tend here is initial simulation end. This value is used to calcu-
C   late growth and fluxes.
                 tend=Tend*86400.
                 tday=tday*3600.
                 dt=dt/it*86400.
C
C ***** Initial values of time variable data
         read(idat,*) tneu,CS,CA,QWd,QWn,humid,temp
C   Transpiration data  ********************************
C tneu: time (d), QWd and QWn: Transpiration day, night ml/h/pl
C    conversion to SI m3/s/plant
         QWd=QWd/1000000./3600.
         QWn=QWn/1000000./3600.
         humid=humid/100.
C
C
C   internal calculation of values:  ************************************
C
C   Leaf-air Conductance*************
C   Calculation of conductance from transpiration, temperature, humidity
C        First: partial pressure of water (Magnus-equation)
C        unit: Pa
         Ew= 6.107*10**(7.5*temp/(273.+temp))*100.
C        The vapour density is (unit kg/m3):
         Rohw= Ew/(461.*(273.+temp))
C        The Conductance for water day and night is:
C        Unit: m/s/plant
         Gdw = 1000.*QWd/(Rohw-humid*Rohw)
         Gnw = 1000.*QWn/(Rohw-humid*Rohw)
         DG=2.57D-5*SQRT(18./XMOLW)
```

```
      DW=2.0D-9*SQRT(32./XMOLW)
C  effective diffusivities
      DWeff=DW*PW**(10/3)/((PA+PW)*(PA+PW))
      DGeff=DG*PA**(10/3)/((PA+PW)*(PA+PW))
C  G units still m/s/plant
      GSn=Gnw*SQRT(18./XMOLW)
      GSd=Gdw*SQRT(18./XMOLW)
C Cuticula Permeance P* is here GC  (unit m/s) *********************
      GC=10**(0.704*PKow-11.2)
      GC=GC/Henry
C     Addition of the air layer resistance  ********
      GA=5.e-3*SQRT(300./XMOLW)
      GC=1/(1/GC+1/GA)
C
C
C  Definition of equilibrium constants to water ********************
C  RCF, SCF and LCF correction exponents z: following Briggs
      zR=0.77
      zL=0.95
      zSt=zR
C  Soil-water
              KS=Roh*Koc*orgC+PW+PA*Henry
C  Root-water
              KR=FatR*Kow**zR+WR
              IF(RCF.NE.0) KR=RCF
C  Air-water
              KAW=Henry
C  Leaf-water
              KL=FatL*Kow**zL+WL
              IF(LCF.NE.0) KL=LCF
C  Stem-water
              KSTXY=FatSt*Kow**zSt+WSt
              IF (RCF.NE.0) KSTXY=RCF
C  Xylem- Water
               IF (TSCF.EQ.0.0) THEN
       TSCF=0.784*exp(-1.*(PKow-1.78)*(PKow-1.78)/2.44)
               END IF
C
C  average linear growth (total simulation time) ***********************
              dVR=(VeR-VaR)/Tend
              dVL=(VeL-VaL)/Tend
              dVSt=(VeSt-VaSt)/Tend
              dVF=(VeF-VaF)/Tend
C  Leaf Area: cm2/cm3 into m2/m3 ********
      AREA=XMA*VL*100.
C
C
C*****************************************************************
C   Optimization of Simulation end
C
C  WARNING !!!
C
C this routine avoids waiting for long time, BUT:
C it also changes the simulation end TEND
C
C  To get the simulation over that time span you wish:
C  Change the time step dt (to those values required !!)
C  However, maybe you've got to wait some time...
C
               If (it.gt.1000000) then
```

```
         Tend=Tend/1000
         write(iout,*)' New end after day: ',Tend/86400.
         write(iout,*)'  and wait a minute ...'
        else if (it.gt.100000) then
         Tend=Tend/500
         write(iout,*)' New end after day: ',Tend/86400.
         write(iout,*)'  and wait a minute ...'
        else if (it.gt.10000) then
         Tend=Tend/50
         write(iout,*)' New end after day: ',Tend/86400.
        else if (it.gt.1000) then
         Tend=Tend/5
         write(iout,*)' New end after day: ',Tend/86400.
         write(iout,*)'  and wait a minute ...'
        else if (it.gt.500) then
         Tend=Tend/5
         write(iout,*)' New end after day: ',Tend/86400.
         write(iout,*)' Simulation Time was changed ! '
         write(iout,*)' Read Program Line 293, please. Thanks '
                 end if
                 Tint=Tend/Nint
C
C Write Head***********************************************
               write(iout,*)'-----------------------------------'
               write(iout,5)
 5    FORMAT('  Days        CRoot     CStem        CLeave    ',
     &' CFruit    CSoil')
               write(ipout,*)text
               write(ipout,5)
C  zero values:
               write(iout,3)th,CR,CST,CL,CF,CS
               write(ipout,3)th,CR,CST,CL,CF,CS
C*********************************************
C  Definition of the initial values of all input time variable values
               CSalt=CS
               CSneu=CS
               CAalt=CA
               CAneu=CA
               QWDneu=QWD
               QWDalt=QWD
               QWNneu=QWN
               QWNalt=QWN
               humidneu=humid
               humidalt=humid
               tempneu=temp
               tempalt=temp
C
C  the time loop:**  set times to zero  *****************
               t=0.0
               tperiod=0.0
               tt=0.0
C
C  let's run ... let's run ... let's run ...****************************
C
 10   t=t+dt
C
C   Read time variable inputs ***********************
C  Time variable Input th in days and linear approximation
C  between input times !!
               th=t/86400.
```

```
                If(th.gt.tneu) then
C change values from new to old *********
                talt=tneu
                CSalt=CSneu
                CAalt=CAneu
                QWNalt=QWNneu
                QWDalt=QWDneu
                HUMIDalt=HUMIDneu
                tempalt=tempneu
                read(idat,*,err=44)tneu,CSneu,CAneu,QWdneu,QWnneu,humidneu,tempn
                goto 45
  44  write(iout,*)' Note: last value of tnew must be larger as Tend !!'
                Goto 99
  45  Continue
        QWdneu=QWdneu/1000000./3600.
        QWnneu=QWnneu/1000000./3600.
        humidneu=humidneu/100.
                end if
C  Factor for linear approximation  ***  =0 at th=talt; =1 at th=tneu
        Factor=(th-talt)/(tneu-talt)
                CS=CSalt-(CSalt-CSneu)*Factor
                CA=CAalt-(CAalt-CAneu)*Factor
                QWD=QWDalt-(QWDalt-QWDneu)*Factor
                QWN=QWNalt-(QWNalt-QWNneu)*Factor
                humid=humidalt-(humidalt-humidneu)*Factor
                temp=tempalt-(tempalt-tempneu)*Factor
C  new conductivities
        Gdw = 1000.*QWd/(Rohw-humid*Rohw)
        Gnw = 1000.*QWn/(Rohw-humid*Rohw)
                GSd=Gdw*SQRT(18./XMOLW)
                GSn=Gnw*SQRT(18./XMOLW)
C
C end of time variable input and linear approximation ***
C
C    The day and night cycle ***
C
                tperiod=tperiod+dt
C
                If(tperiod.le.tday) then
                QW=QWd
                GS=GSd
                Else if(tperiod.gt.86400.) then
                tperiod = 0.0
                else
                QW=QWn
                GS=GSn
                end if
C
C
C*****************************************************************
C
C Growth
C
C  dilution through growth; also Metabolites
                CR=CR*VR/(VR+dVR*dt)
                CXR=CXR*VR/(VR+dVR*dt)
                CL=CL*VL/(VL+dVL*dt)
                CXL=CXL*VL/(VL+dVL*dt)
                CST=CST*VST/(VST+dVSt*dt)
                CXST=CXST*VST/(VST+dVSt*dt)
```

```
                If(VF.eq.0.0) then
                CF=CF
                CXF=CXF
                else
                CF=CF*VF/(VF+dVF*dt)
                CXF=CXF*VF/(VF+dVF*dt)
                end if
C  Volume  growth:
                VR=VR+dVR*dt
                VL=VL+dVL*dt
                VST=VST+dVSt*dt
                VF=VF+dVF*dt
C  Leaf Area: cm2/cm3 into m2/m3
                 AREA=XMA*VL*100.
C  it follows the length of the root:
                XL=VR/(R1*R1*3.1415)
C
C*!***!****!***!***!***!****!**!***!****!****!***!**!***!*
C  The differential equations and their solution   (Main part)
C
C  Definition of terms ************
C Diffusion into roots with water
                T1=DWeff*2.*3.1415927*XL/(DLOG(R2/R1))
C Diffusion into roots via air pores
                T1a=DGeff*2.*3.1415927*XL/DLOG(R2/R1)
C
C**********************
C  Transpiration stream transfer
C  Concentration in xylem before stem
                Cxy=TSCF*CS/KS
C
C  TSR = soil - roots  TL = Stem-leaves , unit kg/s
C  Transport via Transpiration to the roots: Advective transport
                TSR=QW*(1-TSCF)*CS/KS
C
C  Uptake by the Stem, Tstem is Flux into stem
                Tstem=QW*CXy
C Transport to the leaves; transpiration stream is in equilibrium
C  with the stem (after passage of it).
                TL=QW*CSt/KStXy
C
C******************************
C  Uptake into Fruits via Phloem
C  Flux to Fruit. Dry mass*10*2 (Phloem:10% dry mass, Respiration=?)
                QP=(1.-WF)*dVF*10.
C   Leaf to stem; assimilation stream is in equilibrium with the leaf
                TPL=QP*CL/KL
C  Stem to Fruit; assimilation stream is in equilibrium with the stem
                TPS=QP*CST/KSTXY
C   Phloem-concentration = Xylem-concentration in stem
C
C  QWtot is Transpired water in m3; QPtot is assimilat stream
                QWtot=QWtot+QW*dt
                QPtot=QPtot+QP*dt
C
C*****************************************************
C  The final differential equations:
C
C   root (2):
C  change of mass is uptake with transpiration strem (TSR)+
```

```
C  diffusion soil-roots with water (T1*Gradient)+with air(T1a*Gradient)
C  - metabolisation
C
              dCR=TSR/VR+T1*(CS/KS-CR/KR)/VR -XRR*CR
        & +T1a*Henry*(CS/KS-CR/KR)/VR
C
C  stem (St):
C  change of mass is uptake via transpiration stream (Tstem)
C  -metabolization - phloem flux to fruit (TPS)
C  + phloem flux from leaves (TPL) - xylem flux to leaves (TL)
C
              dCST=Tstem/VST - XRSt*CST -TPS/VST +TPL/VST -TL/VSt
C
C   leave (L):
C   change of mass is diffusion into/from air via stomata (GS*Gradient)
C   +- diffusion into/from air via cuticles (Area*GC*Gradient)
C   - metabolization + xylem flux from stem (TL)
C   - phloem flux to stem (TPL)
C
              dCL= GS*(CA-CL*Henry/KL)/VL +AREA*GC*(CA-CL*Henry/KL)/VL - XRL*C
        & +TL/VL -TPL/VL
C
C    Fruit (F):
C    Mass change is flux from stem within phloem - metabolisation
C  if no fruit there: set to zero
              If(VF.eq.0.0) then
              dCF = 0.0
              else
              dCF=TPS/VF-XRF*CF
              end if
C
C   that's all
C
C
C*********************************************************
C   Some balances
C
C  SumQW is sum of flux into plant with the transpiration stream
              SumQW=QW*dt*CS+SumQW
C
C  Transport to the Roots
C  TSR is flux with transpiration stream
              SumTSR=SumTSR+TSR*dt
C   diff is diffusion in water
              Sumdiff=Sumdiff+T1*(CS/KS-CR/KR)*dt
C   diffa is diffusion in air
              Sumdiffa=Sumdiffa+T1a*Henry*(CS/KS-CR/KR)*dt
C
C  QP is phloem flux to the fruits
              SumQP=SumQP+TPS*dt
C  Tstem is xylem flux to the stem
              Sumstem=Sumstem+Tstem*dt
C TL is xylem flux to the leaves
              SumTL=SumTL+TL*dt
C  Volatilization  is VOL
              SumVol= SumVol+GS*(CA-CL*Henry/KL)*dt+
        & AREA*GC*(CA-CL*Henry/KL)*dt
C
C  Integration ******************************************
              CR=CR+dCR*dt
```

```
                    CL=CL+dCL*dt
                    CST=CST+dCST*dt
                    CF=CF+dCF*dt
C*********************************************************
C
C  Optimization of time step: if values below zero occur,
C  then time step is divided by factor 2;
C  this is not an optimal solution, but it works rather satisfying
C  to verify results, select a lower time step than found with this
C  method and see if any differences occur (should not !!).
C
                    If(CR.lt.0.0) then
                    it=it*2
                    Write(iout,*)'  Time step too large, divison by: ', it
                    rewind IDAT
                    close(unit=IPOUT)
                    OPEN(IPOUT,file='plot')
                    goto 100
                    else if(CL.lt.0.0) then
                    it=it*2
                    Write(iout,*)'  Time step too large, divison by: ', it
                    rewind IDAT
                    close(unit=IPOUT)
                    OPEN(IPOUT,file='plot')
                    goto 100
                    else if(CST.lt.0.0) then
                    it=it*2
                    Write(iout,*)'  Time step too large, divison by: ', it
                    rewind IDAT
                    close(unit=IPOUT)
                    OPEN(IPOUT,file='plot')
                    goto 100
                    else if(CF.lt.0.0) then
                    it=it*2
                    Write(iout,*)'  Time step too large, divison by: ', it
                    rewind IDAT
                    close(unit=IPOUT)
                    OPEN(IPOUT,file='plot')
                    goto 100
                    end if
C****************************************************************
C
C  Metabolites
                    CXR=XRR*CR*dt+CXR
                    CXL=XRL*CL*dt+CXL
                    CXSt=XRSt*CST*dt+CXSt
                    CXF=XRF*CF*dt+CXF
C
C**Output on File Plot*******************************************
                    If(tt.ge.tint) then
C
C OUTPUT of PARENT COMPOUND CONCENTRATION
C
C Avoid meaningless Output:
                    If(CR.lt.1.e-37) CR=0.0
                    If(CS.lt.1.e-37) CS=0.0
                    If(CSt.lt.1.e-37) CSt=0.0
                    If(CL.lt.1.e-37) CL=0.0
                    If(CF.lt.1.e-37) CF=0.0
C  th is time in days; C is concentration (mass/volume);
```

```
C  indices see above
                write(iout,3)th,CR,CST,CL,CF,CS
                write(ipout,3)th,CR,CST,CL,CF,CS
 3    Format(' ',6e11.4)
C
                tt=0.0
                end if
C
                tt=tt+dt
                if(t.lt.tend) goto 10
C
C  End of the time loop***!***!***!****!***!****!****!****!****!**!
  99  Continue
C
C**Output on File Result******************************************
                write(iout,5)
                write(iout,35)text
  35  FORMAT(' ',A50)
                write(iout,*) ' Equilibrium constants '
C  KS is partition coefficient soil to water
                write(iout,16) KS
                write(iout1,*) ' Equilibrium constants '
                write(iout1,16) KS
 16   Format('   soil-water   :   ',e12.4)
C
C   KAW/KS is air to soil
                Write(iout,21) KAW/KS,KAW
C   KR/KS is root to soil
                Write(iout,22) KR/KS,KR
C  KL/KS is leaf to soil
                Write(iout,23) KL/KS,KL
C TSCF is transpiration stream to soil solution
                Write(iout,24) TSCF
C same to 'RESULT'
                Write(iout1,21) KAW/KS,KAW
                Write(iout1,22) KR/KS,KR
                Write(iout1,23) KL/KS,KL
                Write(iout1,24) TSCF
 21   Format('   air - soil   :   ',e12.4,' air-water    : ',e12.4)
 22   Format('   root- soil   :   ',e12.4,' root-water   : ',e12.4)
 23   Format('   leaves-soil  :   ',e12.4,' leaves-water: ',e12.4)
 24   Format('   TSCF         :   ',e12.4)
C
C  Output of balancing***********************************
                write(iout,36)t/86400.
                write(iout1,36)t/86400.
  36  FORMAT(' Simulation run time (days) : ',e12.4)
C  A is mass
                AR=CR*VR
                AL=CL*VL
                AST=CST*VST
                AF=CF*VF
C  X is mass of metabolite
                XR=CXR*VR
                XL=CXL*VL
                XST=CXST*VST
                XF=CXF*VF
                 write(iout,25) AR,XR
                 write(iout,26) AST,XSt
                 write(iout,27) AL,XL
```

```
                  write(iout,33) AF,XF
                  write(iout1,25) AR,XR
                  write(iout1,26) AST,XSt
                  write(iout1,27) AL,XL
                  write(iout1,33) AF,XF
 25     FORMAT(' Amount in Roots : ',e11.4,' Metabolites: ',e11.4,' kg')
 26     FORMAT(' Amount in Stems : ',e11.4,' Metabolites: ',e11.4,' kg')
 27     FORMAT(' Amount in Leaves: ',e11.4,' Metabolites: ',e11.4,' kg')
 33     FORMAT(' Amount in Fruits: ',e11.4,' Metabolites: ',e11.4,' kg')
C
                  Write(iout,28)CR,CXR
                  Write(iout,29)CST,CXSt
                  Write(iout,30)CL,CXL
                  Write(iout,31)CF,CXF
                  Write(iout1,28)CR,CXR
                  Write(iout1,29)CST,CXSt
                  Write(iout1,30)CL,CXL
                  Write(iout1,31)CF,CXF
 28     FORMAT(' Conc. in Root   : ',e11.4,' Metabolites: ',e11.4,
     &' kg/m3')
 29     FORMAT(' Conc. in Stem   : ',e11.4,' Metabolites: ',e11.4,
     &' kg/m3')
 30     FORMAT(' Conc. in leaf   : ',e11.4,' Metabolites: ',e11.4,
     &' kg/m3')
 31     FORMAT(' Conc. in fruit  : ',e11.4,' Metabolites: ',e11.4,
     &' kg/m3')
C
                  write(iout,37)QWtot,QPtot
                  write(iout,377)SumTSR
                  write(iout,32)Sumdiff,Sumdiffa
                  write(iout1,37)QWtot,QPtot
                  write(iout1,377)SumTSR
                  write(iout1,32)Sumdiff,Sumdiffa
 37     FORMAT(' Total Transpiration m3 : ',e11.4, ' phloem flux :',
     & e11.4,' m3')
377     FORMAT(' Uptake into roots      : ',e11.4,' with transp. stream')
 32     FORMAT(' Uptake with water diff.: ',e11.4, ' air diff.   :',
     & e11.4,' kg')
C
                  write(iout,34)SumTL,Sumvol
                  write(iout1,34)SumTL,Sumvol
 34     FORMAT(' Transport to leaves    : ',e11.4, ' volatilised :',
     & e11.4,' kg')
C       write(iout,38)Sumstem,SumQP
                  write(iout1,38)SumStem,SumQP
 38     FORMAT(' Transport to stem      : ',e11.4, ' to fruits   :',
     & e11.4,' kg')
                  write(iout,39)GS/AREA,GC
                  write(iout1,39)GS/AREA,GC
 39     FORMAT(' Conductivity of Stomata: ',e11.4, ' of Cuticula :',
     & e11.4, ' m/s')
C
                 If (it.gt.500) then
         write(iout,*)' Simulation Time was changed ! '
         write(iout,*)' Read Program Line 293, please. Thanks '
                 end if
C  Thanks for your interest. intern Units: SI (kg m s)
                 end
```

Appendix B. PLANTX Model Input Parameter Data File Sample

The page immediately following provides an example of the interactive input required to run the PLANTX model. The interactive input consists of the parameters for the specific chemical to be analyzed (TCE in this case). Next is an example of the file PLANT.DAT used as input for the PLANTX model, consisting of the plant, soil, and time variable input parameters. The example file is for the simulation run for a soil TCE concentration of five micrograms per liter, air TCE concentration of 30 ppt, and organic matter content of 1.0%.

```
C This is the standard input file for PLANTX.for
C Root: Mass begin, end (g); Radius (mm), Water, lipid (%), RCF (0=calc)
             31.1    1298.3      1.0          94.2   1.0         0
C Stem: Mass begin, Mass end (g); Water, lipid (%), TSCF (0=calc)
             6.5     135.7           75.6   3.0          0
C Leaf: Mass begin, Mass end (g); Water, lipid (%), LCF (0=calc)
             17.3    361.1           72.7   3.0          0
C Fruit: Mass begin, Mass end (g); Water(%), Leaf Area(cm2/g)
             7.0     292.2           77.0      46.62
C Soil (solution): orgC water pores, air pores (vol/vol) density (g/cm3)
                   0.01     0.3           0.10              1.3
C Times: daytime (h) Simulation End (d) Time step (d),Intervals(#)
             24.0    100                0.01           100
tnew(d) Csoil(kg/m3) Cair(kg/m3) tstd tstn(ml/h) humid(%) temp(C)
 0      0.000005     0.000000       6.3    6.3       50       25
 25     0.000005     0.0000000[illegible]0   37.8   37.8       50       25
 50     0.000005     0.000000030   69.3   69.3       50       25
 75     0.000005     0.000000030  100.9  100.9       50       25
100     0.000005     0.000000030  132.4  132.4       50.      25.
125       0.          0              0      0        50       25

Data for TCE June 1994
tst ist Transpirationsstrom d = Day n = Night
Dokumentation : Stefan Trapp, ab Mai 1992
GSF Mnchen-Neuherberg
spter dann Uni Osnabrck, Angewandte Systemforschung
```

```
C:\PLANTX>plantx
 Model PlantX  by Stefan Trapp

 Scenario in Plant.dat
    Title ? (50 Characters)
Example Interactive Input Parameters
  Molecular weight of the substance g/mol ?
131.39
 logKow of that Substance ?
2.29
 dim.less Henrys Law Const. of that Substance ?
0.397
 Metabolisation Halflife of that Substance (d) ?
2
```

Appendix C. Simulation Results Summary and Key Output Files

The following tables summarize the results for the TCE uptake simulations for the low- and high-organic fraction scenarios. Following the tables are the actual PLANTX output files for those runs that resulted in plant part concentrations surpassing the MCL of five micrograms per liter. The simulation summary result output files for the Hill AFB sites are also included.

Table A.1 Summary of Soil and Corresponding Plant TCE Concentrations for Organic Matter Content = 1.0 % and TCE Air Concentration = 30 ppt (μg/L)				
SOIL	ROOT	STEM	LEAF	FRUIT
0	0	< 1	< 1	< 1
5	4	4	< 1	< 1
6	4	**5**	< 1	< 1
7	**5**	6	< 1	< 1
88	63	70	< 1	2
242	173	192	< 1	**5**
243	174	193	< 1	5
244	174	194	< 1	5
245	175	195	< 1	5
3,000	2,144	2,382	1	62
40,000	28,590	31,770	5	824
43,000	30,730	34,150	5	886
43,034	30,760	34,180	**5**	887
43,035	30,760	34,180	5	887
43,037	30,760	34,180	5	887
44,000	31,450	34,940	5	907
45,000	32,160	35,740	5	928
50,000	35,740	39,710	6	1,031
300,000	214,400	238,200	33	6,184

Table A.2 Summary of Soil and Corresponding Plant TCE Concentrations for Organic Matter Content = 5.0 % and TCE Air Concentration = 30 ppt (μg/L)				
SOIL	ROOT	STEM	LEAF	FRUIT
5	1	1	< 1	< 1
27	4	**5**	< 1	< 1
28	5	5	< 1	< 1
30	**5**	5	< 1	< 1
31	5	6	< 1	< 1
1,057	173	192	< 1	**5**
1,058	173	193	< 1	5
1,059	174	193	< 1	5
1,060	174	193	< 1	5
13,000	2,130	2,367	1	61
30,000	4,916	5,462	1	142
95,000	15,570	17,300	3	449
175,000	28,680	31,860	5	827
185,000	30,310	33,680	5	874
187,000	30,640	34,050	5	884
187,700	30,760	34,170	5	887
187,710	30,760	34,180	**5**	887
187,711	30,760	34,180	5	887
187,712	30,760	34,180	5	887
187,713	30,760	34,180	5	887
187,714	30,760	34,180	5	887
187,715	30,760	34,180	5	887
187,716	30,760	34,180	5	887
187,720	30,760	34,180	5	887
188,000	30,810	34,230	5	888

```
  Model PlantX by Stefan Trapp
OrgC=0.01; CSoil=5 ppb; CAir=30 ppt
  MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
  Equilibrium constants
   soil-water  :     .2129E+01
   air - soil  :     .1865E+00 air-water    :    .3970E+00
   root- soil  :     .7147E+00 root-water   :    .1522E+01
   leaves-soil :     .2452E+01 leaves-water:     .5221E+01
   TSCF        :     .7047E+00
 Simulation run time (days) :    .1000E+03
 Amount in Roots :   .4640E-08 Metabolites:   .8235E-07 kg
 Amount in Stems :   .5389E-09 Metabolites:   .9759E-08 kg
 Amount in Leaves:   .1427E-09 Metabolites:   .2599E-08 kg
 Amount in Fruits:   .3012E-10 Metabolites:   .1006E-08 kg
 Conc. in Root   :   .3574E-05 Metabolites:   .6343E-04 kg/m3
 Conc. in Stem   :   .3971E-05 Metabolites:   .7192E-04 kg/m3
 Conc. in leaf   :   .3951E-06 Metabolites:   .7196E-05 kg/m3
 Conc. in fruit  :   .1031E-06 Metabolites:   .3444E-05 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :   .1154E-06 with transp. stream
 Uptake with water diff.:  -.1991E-09 air diff.    : -.2822E-07 kg
 Transport to leaves    :   .2641E-06 volatilised : -.2613E-06 kg
 Transport to stem      :   .2754E-06 to fruits   :  .1036E-08 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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OrgC=0.01; CSoil=5 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.5000E-05
.1000E+01	.3574E-05	.3788E-05	.3950E-06	.7791E-06	.5000E-05
.2000E+01	.3574E-05	.3815E-05	.3950E-06	.1092E-05	.5000E-05
.3000E+01	.3574E-05	.3836E-05	.3950E-06	.1177E-05	.5000E-05
.4000E+01	.3574E-05	.3851E-05	.3950E-06	.1167E-05	.5000E-05
.5000E+01	.3574E-05	.3864E-05	.3950E-06	.1118E-05	.5000E-05
.6000E+01	.3574E-05	.3875E-05	.3950E-06	.1054E-05	.5000E-05
.7000E+01	.3574E-05	.3884E-05	.3950E-06	.9858E-06	.5000E-05
.8000E+01	.3574E-05	.3891E-05	.3950E-06	.9200E-06	.5000E-05
.9000E+01	.3574E-05	.3898E-05	.3950E-06	.8586E-06	.5000E-05
.1000E+02	.3574E-05	.3903E-05	.3950E-06	.8023E-06	.5000E-05
.1100E+02	.3574E-05	.3908E-05	.3950E-06	.7513E-06	.5000E-05
.1200E+02	.3574E-05	.3912E-05	.3950E-06	.7052E-06	.5000E-05
.1300E+02	.3574E-05	.3916E-05	.3950E-06	.6637E-06	.5000E-05
.1400E+02	.3574E-05	.3920E-05	.3950E-06	.6262E-06	.5000E-05
.1500E+02	.3574E-05	.3923E-05	.3950E-06	.5924E-06	.5000E-05
.1600E+02	.3574E-05	.3926E-05	.3950E-06	.5619E-06	.5000E-05
.1700E+02	.3574E-05	.3928E-05	.3950E-06	.5341E-06	.5000E-05
.1800E+02	.3574E-05	.3931E-05	.3950E-06	.5088E-06	.5000E-05
.1900E+02	.3574E-05	.3933E-05	.3950E-06	.4858E-06	.5000E-05
.2000E+02	.3574E-05	.3935E-05	.3950E-06	.4646E-06	.5000E-05
.2100E+02	.3574E-05	.3936E-05	.3950E-06	.4452E-06	.5000E-05
.2200E+02	.3574E-05	.3938E-05	.3950E-06	.4274E-06	.5000E-05
.2300E+02	.3574E-05	.3940E-05	.3951E-06	.4109E-06	.5000E-05
.2400E+02	.3574E-05	.3941E-05	.3951E-06	.3956E-06	.5000E-05
.2500E+02	.3574E-05	.3943E-05	.3951E-06	.3814E-06	.5000E-05
.2600E+02	.3574E-05	.3944E-05	.3951E-06	.3681E-06	.5000E-05
.2700E+02	.3574E-05	.3945E-05	.3951E-06	.3558E-06	.5000E-05
.2800E+02	.3574E-05	.3946E-05	.3951E-06	.3442E-06	.5000E-05
.2900E+02	.3574E-05	.3947E-05	.3951E-06	.3334E-06	.5000E-05
.3000E+02	.3574E-05	.3948E-05	.3951E-06	.3232E-06	.5000E-05
.3100E+02	.3574E-05	.3949E-05	.3951E-06	.3137E-06	.5000E-05
.3200E+02	.3574E-05	.3950E-05	.3951E-06	.3046E-06	.5000E-05
.3300E+02	.3574E-05	.3951E-05	.3951E-06	.2961E-06	.5000E-05
.3400E+02	.3574E-05	.3952E-05	.3951E-06	.2881E-06	.5000E-05
.3500E+02	.3574E-05	.3953E-05	.3951E-06	.2805E-06	.5000E-05
.3600E+02	.3574E-05	.3953E-05	.3951E-06	.2732E-06	.5000E-05
.3700E+02	.3574E-05	.3954E-05	.3951E-06	.2664E-06	.5000E-05
.3800E+02	.3574E-05	.3955E-05	.3951E-06	.2598E-06	.5000E-05
.3900E+02	.3574E-05	.3955E-05	.3951E-06	.2536E-06	.5000E-05
.4000E+02	.3574E-05	.3956E-05	.3951E-06	.2477E-06	.5000E-05
.4100E+02	.3574E-05	.3956E-05	.3951E-06	.2420E-06	.5000E-05
.4200E+02	.3574E-05	.3957E-05	.3951E-06	.2366E-06	.5000E-05
.4300E+02	.3574E-05	.3958E-05	.3951E-06	.2314E-06	.5000E-05
.4400E+02	.3574E-05	.3958E-05	.3951E-06	.2265E-06	.5000E-05
.4500E+02	.3574E-05	.3959E-05	.3951E-06	.2217E-06	.5000E-05
.4600E+02	.3574E-05	.3959E-05	.3951E-06	.2172E-06	.5000E-05
.4700E+02	.3574E-05	.3959E-05	.3951E-06	.2128E-06	.5000E-05
.4800E+02	.3574E-05	.3960E-05	.3951E-06	.2086E-06	.5000E-05
.4900E+02	.3574E-05	.3960E-05	.3951E-06	.2046E-06	.5000E-05
.5000E+02	.3574E-05	.3961E-05	.3951E-06	.2007E-06	.5000E-05
.5100E+02	.3574E-05	.3961E-05	.3951E-06	.1970E-06	.5000E-05
.5200E+02	.3574E-05	.3961E-05	.3951E-06	.1934E-06	.5000E-05
.5300E+02	.3574E-05	.3962E-05	.3951E-06	.1899E-06	.5000E-05
.5400E+02	.3574E-05	.3962E-05	.3951E-06	.1866E-06	.5000E-05
.5500E+02	.3574E-05	.3963E-05	.3951E-06	.1834E-06	.5000E-05
.5600E+02	.3574E-05	.3963E-05	.3951E-06	.1802E-06	.5000E-05
.5700E+02	.3574E-05	.3963E-05	.3951E-06	.1772E-06	.5000E-05

.5800E+02	.3574E-05	.3964E-05	.3951E-06	.1743E-06	.5000E-05
.5900E+02	.3574E-05	.3964E-05	.3951E-06	.1715E-06	.5000E-05
.6000E+02	.3574E-05	.3964E-05	.3951E-06	.1688E-06	.5000E-05
.6100E+02	.3574E-05	.3964E-05	.3951E-06	.1661E-06	.5000E-05
.6200E+02	.3574E-05	.3965E-05	.3951E-06	.1635E-06	.5000E-05
.6300E+02	.3574E-05	.3965E-05	.3951E-06	.1611E-06	.5000E-05
.6400E+02	.3574E-05	.3965E-05	.3951E-06	.1586E-06	.5000E-05
.6500E+02	.3574E-05	.3965E-05	.3951E-06	.1563E-06	.5000E-05
.6600E+02	.3574E-05	.3966E-05	.3951E-06	.1540E-06	.5000E-05
.6700E+02	.3574E-05	.3966E-05	.3951E-06	.1518E-06	.5000E-05
.6800E+02	.3574E-05	.3966E-05	.3951E-06	.1497E-06	.5000E-05
.6900E+02	.3574E-05	.3966E-05	.3951E-06	.1476E-06	.5000E-05
.7000E+02	.3574E-05	.3967E-05	.3951E-06	.1456E-06	.5000E-05
.7100E+02	.3574E-05	.3967E-05	.3951E-06	.1436E-06	.5000E-05
.7200E+02	.3574E-05	.3967E-05	.3951E-06	.1417E-06	.5000E-05
.7300E+02	.3574E-05	.3967E-05	.3951E-06	.1398E-06	.5000E-05
.7400E+02	.3574E-05	.3967E-05	.3951E-06	.1380E-06	.5000E-05
.7500E+02	.3574E-05	.3968E-05	.3951E-06	.1362E-06	.5000E-05
.7600E+02	.3574E-05	.3968E-05	.3951E-06	.1345E-06	.5000E-05
.7700E+02	.3574E-05	.3968E-05	.3951E-06	.1328E-06	.5000E-05
.7800E+02	.3574E-05	.3968E-05	.3951E-06	.1311E-06	.5000E-05
.7900E+02	.3574E-05	.3968E-05	.3951E-06	.1295E-06	.5000E-05
.8000E+02	.3574E-05	.3969E-05	.3951E-06	.1280E-06	.5000E-05
.8100E+02	.3574E-05	.3969E-05	.3951E-06	.1264E-06	.5000E-05
.8200E+02	.3574E-05	.3969E-05	.3951E-06	.1250E-06	.5000E-05
.8300E+02	.3574E-05	.3969E-05	.3951E-06	.1235E-06	.5000E-05
.8400E+02	.3574E-05	.3969E-05	.3951E-06	.1221E-06	.5000E-05
.8500E+02	.3574E-05	.3969E-05	.3951E-06	.1207E-06	.5000E-05
.8600E+02	.3574E-05	.3969E-05	.3951E-06	.1193E-06	.5000E-05
.8700E+02	.3574E-05	.3970E-05	.3951E-06	.1180E-06	.5000E-05
.8800E+02	.3574E-05	.3970E-05	.3951E-06	.1167E-06	.5000E-05
.8900E+02	.3574E-05	.3970E-05	.3951E-06	.1154E-06	.5000E-05
.9000E+02	.3574E-05	.3970E-05	.3951E-06	.1142E-06	.5000E-05
.9100E+02	.3574E-05	.3970E-05	.3951E-06	.1130E-06	.5000E-05
.9200E+02	.3574E-05	.3970E-05	.3951E-06	.1118E-06	.5000E-05
.9300E+02	.3574E-05	.3970E-05	.3951E-06	.1106E-06	.5000E-05
.9400E+02	.3574E-05	.3971E-05	.3951E-06	.1095E-06	.5000E-05
.9500E+02	.3574E-05	.3971E-05	.3951E-06	.1083E-06	.5000E-05
.9600E+02	.3574E-05	.3971E-05	.3951E-06	.1072E-06	.5000E-05
.9700E+02	.3574E-05	.3971E-05	.3951E-06	.1062E-06	.5000E-05
.9800E+02	.3574E-05	.3971E-05	.3951E-06	.1051E-06	.5000E-05
.9900E+02	.3574E-05	.3971E-05	.3951E-06	.1041E-06	.5000E-05

```
 Model PlantX by Stefan Trapp
OrgC=0.01; CSoil=6ppb; CAir=30 ppt
 MW:    .1314E+03 logKow:    .2290E+01 Henry:   .3970E+00 Halftime:    .2000E+01
 Equilibrium constants
  soil-water  :      .2129E-01
  air - soil  :      .1865E+00 air-water    :    .3970E+00
  root- soil  :      .7147E+00 root-water   :    .1522E+01
  leaves-soil :      .2452E+01 leaves-water:     .5221E+01
  TSCF        :      .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :    .5568E-08 Metabolites:    .9882E-07 kg
 Amount in Stems :    .6467E-09 Metabolites:    .1171E-07 kg
 Amount in Leaves:    .1427E-09 Metabolites:    .2599E-08 kg
 Amount in Fruits:    .3614E-10 Metabolites:    .1207E-08 kg
 Conc. in Root   :    .4288E-05 Metabolites:    .7611E-04 kg/m3
 Conc. in Stem   :    .4765E-05 Metabolites:    .8630E-04 kg/m3
 Conc. in leaf   :    .3952E-06 Metabolites:    .7198E-05 kg/m3
 Conc. in fruit  :    .1237E-06 Metabolites:    .4132E-05 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :    .1385E-06 with transp. stream
 Uptake with water diff.:  -.2390E-09 air diff.    : -.3386E-07 kg
 Transport to leaves    :    .3169E-06 volatilised : -.3141E-06 kg
 Transport to stem      :    .3305E-06 to fruits    :  .1244E-08 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :  .6507E-09 m/s
```

OrgC=0.01; CSoil=6ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.6000E-05
.1000E+01	.4289E-05	.4544E-05	.3951E-06	.9346E-06	.6000E-05
.2000E+01	.4289E-05	.4577E-05	.3951E-06	.1310E-05	.6000E-05
.3000E+01	.4289E-05	.4602E-05	.3951E-06	.1412E-05	.6000E-05
.4000E+01	.4289E-05	.4621E-05	.3951E-06	.1400E-05	.6000E-05
.5000E+01	.4289E-05	.4636E-05	.3951E-06	.1341E-05	.6000E-05
.6000E+01	.4289E-05	.4649E-05	.3951E-06	.1264E-05	.6000E-05
.7000E+01	.4289E-05	.4660E-05	.3951E-06	.1183E-05	.6000E-05
.8000E+01	.4289E-05	.4669E-05	.3951E-06	.1104E-05	.6000E-05
.9000E+01	.4289E-05	.4677E-05	.3951E-06	.1030E-05	.6000E-05
.1000E+02	.4289E-05	.4683E-05	.3952E-06	.9626E-06	.6000E-05
.1100E+02	.4289E-05	.4689E-05	.3952E-06	.9014E-06	.6000E-05
.1200E+02	.4289E-05	.4694E-05	.3952E-06	.8461E-06	.6000E-05
.1300E+02	.4289E-05	.4699E-05	.3952E-06	.7963E-06	.6000E-05
.1400E+02	.4289E-05	.4703E-05	.3952E-06	.7514E-06	.6000E-05
.1500E+02	.4289E-05	.4707E-05	.3952E-06	.7109E-06	.6000E-05
.1600E+02	.4289E-05	.4710E-05	.3952E-06	.6742E-06	.6000E-05
.1700E+02	.4289E-05	.4713E-05	.3952E-06	.6409E-06	.6000E-05
.1800E+02	.4289E-05	.4716E-05	.3952E-06	.6105E-06	.6000E-05
.1900E+02	.4289E-05	.4719E-05	.3952E-06	.5829E-06	.6000E-05
.2000E+02	.4289E-05	.4721E-05	.3952E-06	.5575E-06	.6000E-05
.2100E+02	.4288E-05	.4723E-05	.3952E-06	.5343E-06	.6000E-05
.2200E+02	.4288E-05	.4726E-05	.3952E-06	.5128E-06	.6000E-05
.2300E+02	.4288E-05	.4727E-05	.3952E-06	.4930E-06	.6000E-05
.2400E+02	.4288E-05	.4729E-05	.3952E-06	.4746E-06	.6000E-05
.2500E+02	.4288E-05	.4731E-05	.3952E-06	.4576E-06	.6000E-05
.2600E+02	.4288E-05	.4732E-05	.3952E-06	.4417E-06	.6000E-05
.2700E+02	.4288E-05	.4734E-05	.3952E-06	.4269E-06	.6000E-05
.2800E+02	.4288E-05	.4735E-05	.3952E-06	.4130E-06	.6000E-05
.2900E+02	.4288E-05	.4736E-05	.3952E-06	.4001E-06	.6000E-05
.3000E+02	.4288E-05	.4738E-05	.3952E-06	.3879E-06	.6000E-05
.3100E+02	.4288E-05	.4739E-05	.3952E-06	.3764E-06	.6000E-05
.3200E+02	.4288E-05	.4740E-05	.3952E-06	.3656E-06	.6000E-05
.3300E+02	.4288E-05	.4741E-05	.3952E-06	.3553E-06	.6000E-05
.3400E+02	.4288E-05	.4742E-05	.3952E-06	.3457E-06	.6000E-05
.3500E+02	.4288E-05	.4743E-05	.3952E-06	.3365E-06	.6000E-05
.3600E+02	.4288E-05	.4744E-05	.3952E-06	.3279E-06	.6000E-05
.3700E+02	.4288E-05	.4745E-05	.3952E-06	.3196E-06	.6000E-05
.3800E+02	.4288E-05	.4745E-05	.3952E-06	.3118E-06	.6000E-05
.3900E+02	.4288E-05	.4746E-05	.3952E-06	.3043E-06	.6000E-05
.4000E+02	.4288E-05	.4747E-05	.3952E-06	.2972E-06	.6000E-05
.4100E+02	.4288E-05	.4748E-05	.3952E-06	.2904E-06	.6000E-05
.4200E+02	.4288E-05	.4748E-05	.3952E-06	.2839E-06	.6000E-05
.4300E+02	.4288E-05	.4749E-05	.3952E-06	.2777E-06	.6000E-05
.4400E+02	.4288E-05	.4749E-05	.3952E-06	.2718E-06	.6000E-05
.4500E+02	.4288E-05	.4750E-05	.3952E-06	.2661E-06	.6000E-05
.4600E+02	.4288E-05	.4751E-05	.3952E-06	.2606E-06	.6000E-05
.4700E+02	.4288E-05	.4751E-05	.3952E-06	.2554E-06	.6000E-05
.4800E+02	.4288E-05	.4752E-05	.3952E-06	.2504E-06	.6000E-05
.4900E+02	.4288E-05	.4752E-05	.3952E-06	.2455E-06	.6000E-05
.5000E+02	.4288E-05	.4753E-05	.3952E-06	.2409E-06	.6000E-05
.5100E+02	.4288E-05	.4753E-05	.3952E-06	.2364E-06	.6000E-05
.5200E+02	.4288E-05	.4754E-05	.3952E-06	.2321E-06	.6000E-05
.5300E+02	.4288E-05	.4754E-05	.3952E-06	.2279E-06	.6000E-05
.5400E+02	.4288E-05	.4755E-05	.3952E-06	.2239E-06	.6000E-05
.5500E+02	.4288E-05	.4755E-05	.3952E-06	.2200E-06	.6000E-05
.5600E+02	.4288E-05	.4755E-05	.3952E-06	.2163E-06	.6000E-05
.5700E+02	.4288E-05	.4756E-05	.3952E-06	.2127E-06	.6000E-05

.5800E+02	.4288E-05	.4756E-05	.3952E-06	.2092E-06	.6000E-05
.5900E+02	.4288E-05	.4756E-05	.3952E-06	.2058E-06	.6000E-05
.6000E+02	.4288E-05	.4757E-05	.3952E-06	.2025E-06	.6000E-05
.6100E+02	.4288E-05	.4757E-05	.3952E-06	.1993E-06	.6000E-05
.6200E+02	.4288E-05	.4757E-05	.3952E-06	.1962E-06	.6000E-05
.6300E+02	.4288E-05	.4758E-05	.3952E-06	.1933E-06	.6000E-05
.6400E+02	.4288E-05	.4758E-05	.3952E-06	.1904E-06	.6000E-05
.6500E+02	.4288E-05	.4758E-05	.3952E-06	.1876E-06	.6000E-05
.6600E+02	.4288E-05	.4759E-05	.3952E-06	.1848E-06	.6000E-05
.6700E+02	.4288E-05	.4759E-05	.3952E-06	.1822E-06	.6000E-05
.6800E+02	.4288E-05	.4759E-05	.3952E-06	.1796E-06	.6000E-05
.6900E+02	.4288E-05	.4760E-05	.3952E-06	.1771E-06	.6000E-05
.7000E+02	.4288E-05	.4760E-05	.3952E-06	.1747E-06	.6000E-05
.7100E+02	.4288E-05	.4760E-05	.3952E-06	.1723E-06	.6000E-05
.7200E+02	.4288E-05	.4760E-05	.3952E-06	.1700E-06	.6000E-05
.7300E+02	.4288E-05	.4761E-05	.3952E-06	.1678E-06	.6000E-05
.7400E+02	.4288E-05	.4761E-05	.3952E-06	.1656E-06	.6000E-05
.7500E+02	.4288E-05	.4761E-05	.3952E-06	.1634E-06	.6000E-05
.7600E+02	.4288E-05	.4761E-05	.3952E-06	.1614E-06	.6000E-05
.7700E+02	.4288E-05	.4762E-05	.3952E-06	.1593E-06	.6000E-05
.7800E+02	.4288E-05	.4762E-05	.3952E-06	.1574E-06	.6000E-05
.7900E+02	.4288E-05	.4762E-05	.3952E-06	.1554E-06	.6000E-05
.8000E+02	.4288E-05	.4762E-05	.3952E-06	.1536E-06	.6000E-05
.8100E+02	.4288E-05	.4762E-05	.3952E-06	.1517E-06	.6000E-05
.8200E+02	.4288E-05	.4763E-05	.3952E-06	.1499E-06	.6000E-05
.8300E+02	.4288E-05	.4763E-05	.3952E-06	.1482E-06	.6000E-05
.8400E+02	.4288E-05	.4763E-05	.3952E-06	.1465E-06	.6000E-05
.8500E+02	.4288E-05	.4763E-05	.3952E-06	.1448E-06	.6000E-05
.8600E+02	.4288E-05	.4763E-05	.3952E-06	.1432E-06	.6000E-05
.8700E+02	.4288E-05	.4763E-05	.3952E-06	.1416E-06	.6000E-05
.8800E+02	.4288E-05	.4764E-05	.3952E-06	.1400E-06	.6000E-05
.8900E+02	.4288E-05	.4764E-05	.3952E-06	.1385E-06	.6000E-05
.9000E+02	.4288E-05	.4764E-05	.3952E-06	.1370E-06	.6000E-05
.9100E+02	.4288E-05	.4764E-05	.3952E-06	.1356E-06	.6000E-05
.9200E+02	.4288E-05	.4764E-05	.3952E-06	.1341E-06	.6000E-05
.9300E+02	.4288E-05	.4764E-05	.3952E-06	.1327E-06	.6000E-05
.9400E+02	.4288E-05	.4765E-05	.3952E-06	.1314E-06	.6000E-05
.9500E+02	.4288E-05	.4765E-05	.3952E-06	.1300E-06	.6000E-05
.9600E+02	.4288E-05	.4765E-05	.3952E-06	.1287E-06	.6000E-05
.9700E+02	.4288E-05	.4765E-05	.3952E-06	.1274E-06	.6000E-05
.9800E+02	.4288E-05	.4765E-05	.3952E-06	.1261E-06	.6000E-05
.9900E+02	.4288E-05	.4765E-05	.3952E-06	.1249E-06	.6000E-05

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  Model PlantX by Stefan Trapp
OrgC=0.01; CSoil=7 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:    .2290E+01 Henry:    .3970E+00 Halftime:    .2000E+01
  Equilibrium constants
   soil-water  :      .2129E+01
   air - soil  :      .1865E+00 air-water   :     .3970E+00
   root- soil  :      .7147E+00 root-water  :     .1522E+01
   leaves-soil :      .2452E+01 leaves-water:     .5221E+01
   TSCF        :      .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :    .6496E-08 Metabolites:    .1153E-06 kg
 Amount in Stems :    .7544E-09 Metabolites:    .1366E-07 kg
 Amount in Leaves:    .1427E-09 Metabolites:    .2600E-08 kg
 Amount in Fruits:    .4216E-10 Metabolites:    .1409E-08 kg
 Conc. in Root   :    .5003E-05 Metabolites:    .8880E-04 kg/m3
 Conc. in Stem   :    .5560E-05 Metabolites:    .1007E-03 kg/m3
 Conc. in leaf   :    .3953E-06 Metabolites:    .7200E-05 kg/m3
 Conc. in fruit  :    .1443E-06 Metabolites:    .4821E-05 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :    .1615E-06 with transp. stream
 Uptake with water diff.:   -.2788E-09 air diff.    : -.3950E-07 kg
 Transport to leaves    :    .3697E-06 volatilised : -.3669E-06 kg
 Transport to stem      :    .3855E-06 to fruits    :  .1451E-08 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :  .6507E-09 m/s
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OrgC=0.01; CSoil=7 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.7000E-05
.1000E+01	.5003E-05	.5301E-05	.3952E-06	.1090E-05	.7000E-05
.2000E+01	.5003E-05	.5339E-05	.3952E-06	.1528E-05	.7000E-05
.3000E+01	.5003E-05	.5368E-05	.3952E-06	.1647E-05	.7000E-05
.4000E+01	.5003E-05	.5390E-05	.3952E-06	.1634E-05	.7000E-05
.5000E+01	.5003E-05	.5409E-05	.3952E-06	.1564E-05	.7000E-05
.6000E+01	.5003E-05	.5423E-05	.3952E-06	.1474E-05	.7000E-05
.7000E+01	.5003E-05	.5436E-05	.3953E-06	.1380E-05	.7000E-05
.8000E+01	.5003E-05	.5446E-05	.3953E-06	.1288E-05	.7000E-05
.9000E+01	.5003E-05	.5456E-05	.3953E-06	.1202E-05	.7000E-05
.1000E+02	.5003E-05	.5463E-05	.3953E-06	.1123E-05	.7000E-05
.1100E+02	.5003E-05	.5470E-05	.3953E-06	.1052E-05	.7000E-05
.1200E+02	.5003E-05	.5476E-05	.3953E-06	.9871E-06	.7000E-05
.1300E+02	.5003E-05	.5482E-05	.3953E-06	.9290E-06	.7000E-05
.1400E+02	.5003E-05	.5487E-05	.3953E-06	.8766E-06	.7000E-05
.1500E+02	.5003E-05	.5491E-05	.3953E-06	.8293E-06	.7000E-05
.1600E+02	.5003E-05	.5495E-05	.3953E-06	.7865E-06	.7000E-05
.1700E+02	.5003E-05	.5499E-05	.3953E-06	.7476E-06	.7000E-05
.1800E+02	.5003E-05	.5502E-05	.3953E-06	.7123E-06	.7000E-05
.1900E+02	.5003E-05	.5505E-05	.3953E-06	.6800E-06	.7000E-05
.2000E+02	.5003E-05	.5508E-05	.3953E-06	.6504E-06	.7000E-05
.2100E+02	.5003E-05	.5510E-05	.3953E-06	.6233E-06	.7000E-05
.2200E+02	.5003E-05	.5513E-05	.3953E-06	.5983E-06	.7000E-05
.2300E+02	.5003E-05	.5515E-05	.3953E-06	.5751E-06	.7000E-05
.2400E+02	.5003E-05	.5517E-05	.3953E-06	.5537E-06	.7000E-05
.2500E+02	.5003E-05	.5519E-05	.3953E-06	.5338E-06	.7000E-05
.2600E+02	.5003E-05	.5521E-05	.3953E-06	.5153E-06	.7000E-05
.2700E+02	.5003E-05	.5523E-05	.3953E-06	.4980E-06	.7000E-05
.2800E+02	.5003E-05	.5524E-05	.3953E-06	.4819E-06	.7000E-05
.2900E+02	.5003E-05	.5526E-05	.3953E-06	.4667E-06	.7000E-05
.3000E+02	.5003E-05	.5527E-05	.3953E-06	.4525E-06	.7000E-05
.3100E+02	.5003E-05	.5528E-05	.3953E-06	.4391E-06	.7000E-05
.3200E+02	.5003E-05	.5530E-05	.3953E-06	.4265E-06	.7000E-05
.3300E+02	.5003E-05	.5531E-05	.3953E-06	.4146E-06	.7000E-05
.3400E+02	.5003E-05	.5532E-05	.3953E-06	.4033E-06	.7000E-05
.3500E+02	.5003E-05	.5533E-05	.3953E-06	.3926E-06	.7000E-05
.3600E+02	.5003E-05	.5534E-05	.3953E-06	.3825E-06	.7000E-05
.3700E+02	.5003E-05	.5535E-05	.3953E-06	.3729E-06	.7000E-05
.3800E+02	.5003E-05	.5536E-05	.3953E-06	.3637E-06	.7000E-05
.3900E+02	.5003E-05	.5537E-05	.3953E-06	.3550E-06	.7000E-05
.4000E+02	.5003E-05	.5538E-05	.3953E-06	.3467E-06	.7000E-05
.4100E+02	.5003E-05	.5539E-05	.3953E-06	.3388E-06	.7000E-05
.4200E+02	.5003E-05	.5539E-05	.3953E-06	.3312E-06	.7000E-05
.4300E+02	.5003E-05	.5540E-05	.3953E-06	.3240E-06	.7000E-05
.4400E+02	.5003E-05	.5541E-05	.3953E-06	.3171E-06	.7000E-05
.4500E+02	.5003E-05	.5542E-05	.3953E-06	.3104E-06	.7000E-05
.4600E+02	.5003E-05	.5542E-05	.3953E-06	.3041E-06	.7000E-05
.4700E+02	.5003E-05	.5543E-05	.3953E-06	.2980E-06	.7000E-05
.4800E+02	.5003E-05	.5544E-05	.3953E-06	.2921E-06	.7000E-05
.4900E+02	.5003E-05	.5544E-05	.3953E-06	.2864E-06	.7000E-05
.5000E+02	.5003E-05	.5545E-05	.3953E-06	.2810E-06	.7000E-05
.5100E+02	.5003E-05	.5545E-05	.3953E-06	.2758E-06	.7000E-05
.5200E+02	.5003E-05	.5546E-05	.3953E-06	.2708E-06	.7000E-05
.5300E+02	.5003E-05	.5546E-05	.3953E-06	.2659E-06	.7000E-05
.5400E+02	.5003E-05	.5547E-05	.3953E-06	.2612E-06	.7000E-05
.5500E+02	.5003E-05	.5547E-05	.3953E-06	.2567E-06	.7000E-05
.5600E+02	.5003E-05	.5548E-05	.3953E-06	.2523E-06	.7000E-05
.5700E+02	.5003E-05	.5548E-05	.3953E-06	.2481E-06	.7000E-05

.5800E+02	.5003E-05	.5549E-05	.3953E-06	.2440E-06	.7000E-05
.5900E+02	.5003E-05	.5549E-05	.3953E-06	.2401E-06	.7000E-05
.6000E+02	.5003E-05	.5550E-05	.3953E-06	.2362E-06	.7000E-05
.6100E+02	.5003E-05	.5550E-05	.3953E-06	.2325E-06	.7000E-05
.6200E+02	.5003E-05	.5550E-05	.3953E-06	.2290E-06	.7000E-05
.6300E+02	.5003E-05	.5551E-05	.3953E-06	.2255E-06	.7000E-05
.6400E+02	.5003E-05	.5551E-05	.3953E-06	.2221E-06	.7000E-05
.6500E+02	.5003E-05	.5551E-05	.3953E-06	.2188E-06	.7000E-05
.6600E+02	.5003E-05	.5552E-05	.3953E-06	.2156E-06	.7000E-05
.6700E+02	.5003E-05	.5552E-05	.3953E-06	.2125E-06	.7000E-05
.6800E+02	.5003E-05	.5552E-05	.3953E-06	.2095E-06	.7000E-05
.6900E+02	.5003E-05	.5553E-05	.3953E-06	.2066E-06	.7000E-05
.7000E+02	.5003E-05	.5553E-05	.3953E-06	.2038E-06	.7000E-05
.7100E+02	.5003E-05	.5553E-05	.3953E-06	.2010E-06	.7000E-05
.7200E+02	.5003E-05	.5554E-05	.3953E-06	.1983E-06	.7000E-05
.7300E+02	.5003E-05	.5554E-05	.3953E-06	.1957E-06	.7000E-05
.7400E+02	.5003E-05	.5554E-05	.3953E-06	.1932E-06	.7000E-05
.7500E+02	.5003E-05	.5555E-05	.3953E-06	.1907E-06	.7000E-05
.7600E+02	.5003E-05	.5555E-05	.3953E-06	.1883E-06	.7000E-05
.7700E+02	.5003E-05	.5555E-05	.3953E-06	.1859E-06	.7000E-05
.7800E+02	.5003E-05	.5555E-05	.3953E-06	.1836E-06	.7000E-05
.7900E+02	.5003E-05	.5556E-05	.3953E-06	.1814E-06	.7000E-05
.8000E+02	.5003E-05	.5556E-05	.3953E-06	.1792E-06	.7000E-05
.8100E+02	.5003E-05	.5556E-05	.3953E-06	.1770E-06	.7000E-05
.8200E+02	.5003E-05	.5556E-05	.3953E-06	.1749E-06	.7000E-05
.8300E+02	.5003E-05	.5556E-05	.3953E-06	.1729E-06	.7000E-05
.8400E+02	.5003E-05	.5557E-05	.3953E-06	.1709E-06	.7000E-05
.8500E+02	.5003E-05	.5557E-05	.3953E-06	.1690E-06	.7000E-05
.8600E+02	.5003E-05	.5557E-05	.3953E-06	.1671E-06	.7000E-05
.8700E+02	.5003E-05	.5557E-05	.3953E-06	.1652E-06	.7000E-05
.8800E+02	.5003E-05	.5557E-05	.3953E-06	.1634E-06	.7000E-05
.8900E+02	.5003E-05	.5558E-05	.3953E-06	.1616E-06	.7000E-05
.9000E+02	.5003E-05	.5558E-05	.3953E-06	.1598E-06	.7000E-05
.9100E+02	.5003E-05	.5558E-05	.3953E-06	.1581E-06	.7000E-05
.9200E+02	.5003E-05	.5558E-05	.3953E-06	.1565E-06	.7000E-05
.9300E+02	.5003E-05	.5558E-05	.3953E-06	.1548E-06	.7000E-05
.9400E+02	.5003E-05	.5559E-05	.3953E-06	.1532E-06	.7000E-05
.9500E+02	.5003E-05	.5559E-05	.3953E-06	.1517E-06	.7000E-05
.9600E+02	.5003E-05	.5559E-05	.3953E-06	.1501E-06	.7000E-05
.9700E+02	.5003E-05	.5559E-05	.3953E-06	.1486E-06	.7000E-05
.9800E+02	.5003E-05	.5559E-05	.3953E-06	.1472E-06	.7000E-05
.9900E+02	.5003E-05	.5559E-05	.3953E-06	.1457E-06	.7000E-05

```
 Model PlantX by Stefan Trapp
OrgC=0.01; CSoil=242 ppb; CAir=30 ppt
 MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
 Equilibrium constants
  soil-water   :       .2129E+01
  air - soil   :       .1865E+00 air-water    :     .3970E+00
  root- soil   :       .7147E+00 root-water   :     .1522E+01
  leaves-soil  :       .2452E+01 leaves-water:      .5221E+01
  TSCF         :       .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :     .2246E-06 Metabolites:    .3986E-05 kg
 Amount in Stems :     .2608E-07 Metabolites:    .4723E-06 kg
 Amount in Leaves:     .1518E-09 Metabolites:    .2764E-08 kg
 Amount in Fruits:     .1458E-08 Metabolites:    .4869E-07 kg
 Conc. in Root    :    .1730E-03 Metabolites:    .3070E-02 kg/m3
 Conc. in Stem    :    .1922E-03 Metabolites:    .3480E-02 kg/m3
 Conc. in leaf    :    .4204E-06 Metabolites:    .7656E-05 kg/m3
 Conc. in fruit   :    .4988E-05 Metabolites:    .1666E-03 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :    .5585E-05 with transp. stream
 Uptake with water diff.:  -.9638E-08 air diff.    : -.1366E-05 kg
 Transport to leaves    :    .1278E-04 volatilised : -.1278E-04 kg
 Transport to stem      :    .1333E-04 to fruits    :   .5015E-07 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :   .6507E-09 m/s
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OrgC=0.01; CSoil=242 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.2420E-03
.1000E+01	.1730E-03	.1830E-03	.4192E-06	.3764E-04	.2420E-03
.2000E+01	.1730E-03	.1844E-03	.4194E-06	.5278E-04	.2420E-03
.3000E+01	.1730E-03	.1854E-03	.4195E-06	.5689E-04	.2420E-03
.4000E+01	.1730E-03	.1862E-03	.4196E-06	.5642E-04	.2420E-03
.5000E+01	.1730E-03	.1869E-03	.4197E-06	.5404E-04	.2420E-03
.6000E+01	.1730E-03	.1874E-03	.4198E-06	.5093E-04	.2420E-03
.7000E+01	.1730E-03	.1878E-03	.4198E-06	.4766E-04	.2420E-03
.8000E+01	.1730E-03	.1882E-03	.4199E-06	.4449E-04	.2420E-03
.9000E+01	.1730E-03	.1885E-03	.4199E-06	.4152E-04	.2420E-03
.1000E+02	.1730E-03	.1888E-03	.4200E-06	.3880E-04	.2420E-03
.1100E+02	.1730E-03	.1890E-03	.4200E-06	.3633E-04	.2420E-03
.1200E+02	.1730E-03	.1893E-03	.4200E-06	.3411E-04	.2420E-03
.1300E+02	.1730E-03	.1894E-03	.4200E-06	.3210E-04	.2420E-03
.1400E+02	.1730E-03	.1896E-03	.4201E-06	.3029E-04	.2420E-03
.1500E+02	.1730E-03	.1898E-03	.4201E-06	.2866E-04	.2420E-03
.1600E+02	.1730E-03	.1899E-03	.4201E-06	.2718E-04	.2420E-03
.1700E+02	.1730E-03	.1900E-03	.4201E-06	.2584E-04	.2420E-03
.1800E+02	.1730E-03	.1902E-03	.4201E-06	.2462E-04	.2420E-03
.1900E+02	.1730E-03	.1903E-03	.4202E-06	.2350E-04	.2420E-03
.2000E+02	.1730E-03	.1904E-03	.4202E-06	.2248E-04	.2420E-03
.2100E+02	.1730E-03	.1905E-03	.4202E-06	.2154E-04	.2420E-03
.2200E+02	.1730E-03	.1905E-03	.4202E-06	.2068E-04	.2420E-03
.2300E+02	.1730E-03	.1906E-03	.4202E-06	.1988E-04	.2420E-03
.2400E+02	.1730E-03	.1907E-03	.4202E-06	.1914E-04	.2420E-03
.2500E+02	.1730E-03	.1908E-03	.4202E-06	.1845E-04	.2420E-03
.2600E+02	.1730E-03	.1908E-03	.4202E-06	.1781E-04	.2420E-03
.2700E+02	.1730E-03	.1909E-03	.4202E-06	.1721E-04	.2420E-03
.2800E+02	.1730E-03	.1909E-03	.4202E-06	.1666E-04	.2420E-03
.2900E+02	.1730E-03	.1910E-03	.4203E-06	.1613E-04	.2420E-03
.3000E+02	.1730E-03	.1910E-03	.4203E-06	.1564E-04	.2420E-03
.3100E+02	.1730E-03	.1911E-03	.4203E-06	.1518E-04	.2420E-03
.3200E+02	.1730E-03	.1911E-03	.4203E-06	.1474E-04	.2420E-03
.3300E+02	.1730E-03	.1912E-03	.4203E-06	.1433E-04	.2420E-03
.3400E+02	.1730E-03	.1912E-03	.4203E-06	.1394E-04	.2420E-03
.3500E+02	.1730E-03	.1913E-03	.4203E-06	.1357E-04	.2420E-03
.3600E+02	.1730E-03	.1913E-03	.4203E-06	.1322E-04	.2420E-03
.3700E+02	.1730E-03	.1913E-03	.4203E-06	.1289E-04	.2420E-03
.3800E+02	.1730E-03	.1914E-03	.4203E-06	.1257E-04	.2420E-03
.3900E+02	.1730E-03	.1914E-03	.4203E-06	.1227E-04	.2420E-03
.4000E+02	.1730E-03	.1914E-03	.4203E-06	.1198E-04	.2420E-03
.4100E+02	.1730E-03	.1915E-03	.4203E-06	.1171E-04	.2420E-03
.4200E+02	.1730E-03	.1915E-03	.4203E-06	.1145E-04	.2420E-03
.4300E+02	.1730E-03	.1915E-03	.4203E-06	.1120E-04	.2420E-03
.4400E+02	.1730E-03	.1915E-03	.4203E-06	.1096E-04	.2420E-03
.4500E+02	.1730E-03	.1916E-03	.4203E-06	.1073E-04	.2420E-03
.4600E+02	.1730E-03	.1916E-03	.4203E-06	.1051E-04	.2420E-03
.4700E+02	.1730E-03	.1916E-03	.4203E-06	.1030E-04	.2420E-03
.4800E+02	.1730E-03	.1916E-03	.4203E-06	.1010E-04	.2420E-03
.4900E+02	.1730E-03	.1916E-03	.4203E-06	.9901E-05	.2420E-03
.5000E+02	.1730E-03	.1917E-03	.4203E-06	.9714E-05	.2420E-03
.5100E+02	.1730E-03	.1917E-03	.4203E-06	.9533E-05	.2420E-03
.5200E+02	.1730E-03	.1917E-03	.4204E-06	.9359E-05	.2420E-03
.5300E+02	.1730E-03	.1917E-03	.4204E-06	.9191E-05	.2420E-03
.5400E+02	.1730E-03	.1917E-03	.4204E-06	.9029E-05	.2420E-03
.5500E+02	.1730E-03	.1918E-03	.4204E-06	.8873E-05	.2420E-03
.5600E+02	.1730E-03	.1918E-03	.4204E-06	.8722E-05	.2420E-03
.5700E+02	.1730E-03	.1918E-03	.4204E-06	.8576E-05	.2420E-03

.5800E+02	.1730E-03	.1918E-03	.4204E-06	.8435E-05	.2420E-03
.5900E+02	.1730E-03	.1918E-03	.4204E-06	.8299E-05	.2420E-03
.6000E+02	.1730E-03	.1918E-03	.4204E-06	.8166E-05	.2420E-03
.6100E+02	.1730E-03	.1918E-03	.4204E-06	.8038E-05	.2420E-03
.6200E+02	.1730E-03	.1919E-03	.4204E-06	.7914E-05	.2420E-03
.6300E+02	.1730E-03	.1919E-03	.4204E-06	.7794E-05	.2420E-03
.6400E+02	.1730E-03	.1919E-03	.4204E-06	.7677E-05	.2420E-03
.6500E+02	.1730E-03	.1919E-03	.4204E-06	.7564E-05	.2420E-03
.6600E+02	.1730E-03	.1919E-03	.4204E-06	.7454E-05	.2420E-03
.6700E+02	.1730E-03	.1919E-03	.4204E-06	.7347E-05	.2420E-03
.6800E+02	.1730E-03	.1919E-03	.4204E-06	.7243E-05	.2420E-03
.6900E+02	.1730E-03	.1919E-03	.4204E-06	.7143E-05	.2420E-03
.7000E+02	.1730E-03	.1920E-03	.4204E-06	.7044E-05	.2420E-03
.7100E+02	.1730E-03	.1920E-03	.4204E-06	.6949E-05	.2420E-03
.7200E+02	.1730E-03	.1920E-03	.4204E-06	.6856E-05	.2420E-03
.7300E+02	.1730E-03	.1920E-03	.4204E-06	.6766E-05	.2420E-03
.7400E+02	.1730E-03	.1920E-03	.4204E-06	.6677E-05	.2420E-03
.7500E+02	.1730E-03	.1920E-03	.4204E-06	.6592E-05	.2420E-03
.7600E+02	.1730E-03	.1920E-03	.4204E-06	.6508E-05	.2420E-03
.7700E+02	.1730E-03	.1920E-03	.4204E-06	.6426E-05	.2420E-03
.7800E+02	.1730E-03	.1920E-03	.4204E-06	.6347E-05	.2420E-03
.7900E+02	.1730E-03	.1920E-03	.4204E-06	.6269E-05	.2420E-03
.8000E+02	.1730E-03	.1921E-03	.4204E-06	.6193E-05	.2420E-03
.8100E+02	.1730E-03	.1921E-03	.4204E-06	.6119E-05	.2420E-03
.8200E+02	.1730E-03	.1921E-03	.4204E-06	.6047E-05	.2420E-03
.8300E+02	.1730E-03	.1921E-03	.4204E-06	.5977E-05	.2420E-03
.8400E+02	.1730E-03	.1921E-03	.4204E-06	.5908E-05	.2420E-03
.8500E+02	.1730E-03	.1921E-03	.4204E-06	.5841E-05	.2420E-03
.8600E+02	.1730E-03	.1921E-03	.4204E-06	.5775E-05	.2420E-03
.8700E+02	.1730E-03	.1921E-03	.4204E-06	.5710E-05	.2420E-03
.8800E+02	.1730E-03	.1921E-03	.4204E-06	.5648E-05	.2420E-03
.8900E+02	.1730E-03	.1921E-03	.4204E-06	.5586E-05	.2420E-03
.9000E+02	.1730E-03	.1921E-03	.4204E-06	.5526E-05	.2420E-03
.9100E+02	.1730E-03	.1921E-03	.4204E-06	.5467E-05	.2420E-03
.9200E+02	.1730E-03	.1921E-03	.4204E-06	.5409E-05	.2420E-03
.9300E+02	.1730E-03	.1921E-03	.4204E-06	.5353E-05	.2420E-03
.9400E+02	.1730E-03	.1922E-03	.4204E-06	.5297E-05	.2420E-03
.9500E+02	.1730E-03	.1922E-03	.4204E-06	.5243E-05	.2420E-03
.9600E+02	.1730E-03	.1922E-03	.4204E-06	.5190E-05	.2420E-03
.9700E+02	.1730E-03	.1922E-03	.4204E-06	.5138E-05	.2420E-03
.9800E+02	.1730E-03	.1922E-03	.4204E-06	.5087E-05	.2420E-03
.9900E+02	.1730E-03	.1922E-03	.4204E-06	.5037E-05	.2420E-03

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 Model PlantX by Stefan Trapp
OrgC=0.01; CSoil=43034 ppb; CAir=30 ppt
 MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
 Equilibrium constants
  soil-water  :      .2129E+01
  air - soil  :      .1865E+00 air-water   :    .3970E+00
  root- soil  :      .7147E+00 root-water  :    .1522E+01
  leaves-soil :      .2452E+01 leaves-water:    .5221E+01
  TSCF        :      .7047E+00
 Simulation run time (days) :    .1000E+03
 Amount in Roots :   .3993E-04 Metabolites:   .7087E-03 kg
 Amount in Stems :   .4638E-05 Metabolites:   .8398E-04 kg
 Amount in Leaves:   .1805E-08 Metabolites:   .3271E-07 kg
 Amount in Fruits:   .2592E-06 Metabolites:   .8658E-05 kg
 Conc. in Root   :   .3076E-01 Metabolites:   .5459E+00 kg/m3
 Conc. in Stem   :   .3418E-01 Metabolites:   .6189E+00 kg/m3
 Conc. in leaf   :   .5000E-05 Metabolites:   .9058E-04 kg/m3
 Conc. in fruit  :   .8870E-03 Metabolites:   .2963E-01 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :   .9931E-03 with transp. stream
 Uptake with water diff.:  -.1714E-05 air diff.   : -.2429E-03 kg
 Transport to leaves    :   .2273E-02 volatilised : -.2273E-02 kg
 Transport to stem      :   .2370E-02 to fruits   :  .8917E-05 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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OrgC=0.01; CSoil=43034 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.4303E-01
.1000E+01	.3076E-01	.3255E-01	.4780E-05	.6694E-02	.4303E-01
.2000E+01	.3076E-01	.3279E-01	.4813E-05	.9385E-02	.4303E-01
.3000E+01	.3076E-01	.3297E-01	.4837E-05	.1012E-01	.4303E-01
.4000E+01	.3076E-01	.3311E-01	.4856E-05	.1003E-01	.4303E-01
.5000E+01	.3076E-01	.3323E-01	.4872E-05	.9609E-02	.4303E-01
.6000E+01	.3076E-01	.3332E-01	.4884E-05	.9057E-02	.4303E-01
.7000E+01	.3076E-01	.3340E-01	.4895E-05	.8475E-02	.4303E-01
.8000E+01	.3076E-01	.3346E-01	.4904E-05	.7911E-02	.4303E-01
.9000E+01	.3076E-01	.3352E-01	.4911E-05	.7383E-02	.4303E-01
.1000E+02	.3076E-01	.3357E-01	.4918E-05	.6900E-02	.4303E-01
.1100E+02	.3076E-01	.3362E-01	.4924E-05	.6461E-02	.4303E-01
.1200E+02	.3076E-01	.3365E-01	.4929E-05	.6065E-02	.4303E-01
.1300E+02	.3076E-01	.3369E-01	.4934E-05	.5708E-02	.4303E-01
.1400E+02	.3076E-01	.3372E-01	.4938E-05	.5386E-02	.4303E-01
.1500E+02	.3076E-01	.3375E-01	.4942E-05	.5096E-02	.4303E-01
.1600E+02	.3076E-01	.3377E-01	.4945E-05	.4833E-02	.4303E-01
.1700E+02	.3076E-01	.3379E-01	.4948E-05	.4594E-02	.4303E-01
.1800E+02	.3076E-01	.3381E-01	.4951E-05	.4377E-02	.4303E-01
.1900E+02	.3076E-01	.3383E-01	.4953E-05	.4179E-02	.4303E-01
.2000E+02	.3076E-01	.3385E-01	.4956E-05	.3997E-02	.4303E-01
.2100E+02	.3076E-01	.3387E-01	.4958E-05	.3830E-02	.4303E-01
.2200E+02	.3076E-01	.3388E-01	.4960E-05	.3677E-02	.4303E-01
.2300E+02	.3076E-01	.3390E-01	.4962E-05	.3535E-02	.4303E-01
.2400E+02	.3076E-01	.3391E-01	.4964E-05	.3403E-02	.4303E-01
.2500E+02	.3076E-01	.3392E-01	.4965E-05	.3281E-02	.4303E-01
.2600E+02	.3076E-01	.3393E-01	.4967E-05	.3167E-02	.4303E-01
.2700E+02	.3076E-01	.3394E-01	.4968E-05	.3061E-02	.4303E-01
.2800E+02	.3076E-01	.3395E-01	.4970E-05	.2962E-02	.4303E-01
.2900E+02	.3076E-01	.3396E-01	.4971E-05	.2869E-02	.4303E-01
.3000E+02	.3076E-01	.3397E-01	.4972E-05	.2781E-02	.4303E-01
.3100E+02	.3076E-01	.3398E-01	.4973E-05	.2699E-02	.4303E-01
.3200E+02	.3076E-01	.3399E-01	.4974E-05	.2621E-02	.4303E-01
.3300E+02	.3076E-01	.3400E-01	.4975E-05	.2548E-02	.4303E-01
.3400E+02	.3076E-01	.3400E-01	.4976E-05	.2479E-02	.4303E-01
.3500E+02	.3076E-01	.3401E-01	.4977E-05	.2413E-02	.4303E-01
.3600E+02	.3076E-01	.3402E-01	.4978E-05	.2351E-02	.4303E-01
.3700E+02	.3076E-01	.3402E-01	.4979E-05	.2292E-02	.4303E-01
.3800E+02	.3076E-01	.3403E-01	.4980E-05	.2236E-02	.4303E-01
.3900E+02	.3076E-01	.3403E-01	.4980E-05	.2182E-02	.4303E-01
.4000E+02	.3076E-01	.3404E-01	.4981E-05	.2131E-02	.4303E-01
.4100E+02	.3076E-01	.3404E-01	.4982E-05	.2082E-02	.4303E-01
.4200E+02	.3076E-01	.3405E-01	.4983E-05	.2036E-02	.4303E-01
.4300E+02	.3076E-01	.3405E-01	.4983E-05	.1991E-02	.4303E-01
.4400E+02	.3076E-01	.3406E-01	.4984E-05	.1949E-02	.4303E-01
.4500E+02	.3076E-01	.3406E-01	.4984E-05	.1908E-02	.4303E-01
.4600E+02	.3076E-01	.3407E-01	.4985E-05	.1869E-02	.4303E-01
.4700E+02	.3076E-01	.3407E-01	.4985E-05	.1831E-02	.4303E-01
.4800E+02	.3076E-01	.3408E-01	.4986E-05	.1795E-02	.4303E-01
.4900E+02	.3076E-01	.3408E-01	.4986E-05	.1761E-02	.4303E-01
.5000E+02	.3076E-01	.3408E-01	.4987E-05	.1727E-02	.4303E-01
.5100E+02	.3076E-01	.3409E-01	.4987E-05	.1695E-02	.4303E-01
.5200E+02	.3076E-01	.3409E-01	.4988E-05	.1664E-02	.4303E-01
.5300E+02	.3076E-01	.3409E-01	.4988E-05	.1634E-02	.4303E-01
.5400E+02	.3076E-01	.3410E-01	.4989E-05	.1606E-02	.4303E-01
.5500E+02	.3076E-01	.3410E-01	.4989E-05	.1578E-02	.4303E-01
.5600E+02	.3076E-01	.3410E-01	.4990E-05	.1551E-02	.4303E-01
.5700E+02	.3076E-01	.3411E-01	.4990E-05	.1525E-02	.4303E-01

.5800E+02	.3076E-01	.3411E-01	.4990E-05	.1500E-02	.4303E-01
.5900E+02	.3076E-01	.3411E-01	.4991E-05	.1476E-02	.4303E-01
.6000E+02	.3076E-01	.3411E-01	.4991E-05	.1452E-02	.4303E-01
.6100E+02	.3076E-01	.3412E-01	.4991E-05	.1429E-02	.4303E-01
.6200E+02	.3076E-01	.3412E-01	.4992E-05	.1407E-02	.4303E-01
.6300E+02	.3076E-01	.3412E-01	.4992E-05	.1386E-02	.4303E-01
.6400E+02	.3076E-01	.3412E-01	.4992E-05	.1365E-02	.4303E-01
.6500E+02	.3076E-01	.3413E-01	.4993E-05	.1345E-02	.4303E-01
.6600E+02	.3076E-01	.3413E-01	.4993E-05	.1326E-02	.4303E-01
.6700E+02	.3076E-01	.3413E-01	.4993E-05	.1307E-02	.4303E-01
.6800E+02	.3076E-01	.3413E-01	.4994E-05	.1288E-02	.4303E-01
.6900E+02	.3076E-01	.3413E-01	.4994E-05	.1270E-02	.4303E-01
.7000E+02	.3076E-01	.3414E-01	.4994E-05	.1253E-02	.4303E-01
.7100E+02	.3076E-01	.3414E-01	.4994E-05	.1236E-02	.4303E-01
.7200E+02	.3076E-01	.3414E-01	.4995E-05	.1219E-02	.4303E-01
.7300E+02	.3076E-01	.3414E-01	.4995E-05	.1203E-02	.4303E-01
.7400E+02	.3076E-01	.3414E-01	.4995E-05	.1187E-02	.4303E-01
.7500E+02	.3076E-01	.3414E-01	.4995E-05	.1172E-02	.4303E-01
.7600E+02	.3076E-01	.3415E-01	.4996E-05	.1157E-02	.4303E-01
.7700E+02	.3076E-01	.3415E-01	.4996E-05	.1143E-02	.4303E-01
.7800E+02	.3076E-01	.3415E-01	.4996E-05	.1129E-02	.4303E-01
.7900E+02	.3076E-01	.3415E-01	.4996E-05	.1115E-02	.4303E-01
.8000E+02	.3076E-01	.3415E-01	.4996E-05	.1101E-02	.4303E-01
.8100E+02	.3076E-01	.3415E-01	.4997E-05	.1088E-02	.4303E-01
.8200E+02	.3076E-01	.3416E-01	.4997E-05	.1075E-02	.4303E-01
.8300E+02	.3076E-01	.3416E-01	.4997E-05	.1063E-02	.4303E-01
.8400E+02	.3076E-01	.3416E-01	.4997E-05	.1051E-02	.4303E-01
.8500E+02	.3076E-01	.3416E-01	.4997E-05	.1039E-02	.4303E-01
.8600E+02	.3076E-01	.3416E-01	.4997E-05	.1027E-02	.4303E-01
.8700E+02	.3076E-01	.3416E-01	.4998E-05	.1015E-02	.4303E-01
.8800E+02	.3076E-01	.3416E-01	.4998E-05	.1004E-02	.4303E-01
.8900E+02	.3076E-01	.3416E-01	.4998E-05	.9933E-03	.4303E-01
.9000E+02	.3076E-01	.3417E-01	.4998E-05	.9826E-03	.4303E-01
.9100E+02	.3076E-01	.3417E-01	.4998E-05	.9721E-03	.4303E-01
.9200E+02	.3076E-01	.3417E-01	.4998E-05	.9619E-03	.4303E-01
.9300E+02	.3076E-01	.3417E-01	.4999E-05	.9518E-03	.4303E-01
.9400E+02	.3076E-01	.3417E-01	.4999E-05	.9420E-03	.4303E-01
.9500E+02	.3076E-01	.3417E-01	.4999E-05	.9324E-03	.4303E-01
.9600E+02	.3076E-01	.3417E-01	.4999E-05	.9229E-03	.4303E-01
.9700E+02	.3076E-01	.3417E-01	.4999E-05	.9137E-03	.4303E-01
.9800E+02	.3076E-01	.3417E-01	.4999E-05	.9046E-03	.4303E-01
.9900E+02	.3076E-01	.3418E-01	.4999E-05	.8957E-03	.4303E-01

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  Model PlantX by Stefan Trapp
OrgC=0.05; CSoil=5 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:   .2290E+01 Henry:    .3970E+00 Halftime:    .2000E-01
  Equilibrium constants
   soil-water   :      .9287E+01
   air - soil   :      .4275E-01 air-water    :     .3970E+00
   root- soil   :      .1639E+00 root-water   :     .1522E+01
   leaves-soil  :      .5621E+00 leaves-water:      .5221E+01
   TSCF         :      .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :    .1064E-08 Metabolites:    .1888E-07 kg
 Amount in Stems :    .1236E-09 Metabolites:    .2239E-08 kg
 Amount in Leaves:    .1425E-09 Metabolites:    .2596E-08 kg
 Amount in Fruits:    .6907E-11 Metabolites:    .2309E-09 kg
 Conc. in Root   :    .8193E-06 Metabolites:    .1454E-04 kg/m3
 Conc. in Stem   :    .9107E-06 Metabolites:    .1650E-04 kg/m3
 Conc. in leaf   :    .3946E-06 Metabolites:    .7189E-05 kg/m3
 Conc. in fruit  :    .2364E-07 Metabolites:    .7903E-06 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :    .2645E-07 with transp. stream
 Uptake with water diff.:  -.4565E-10 air diff.   : -.6469E-08 kg
 Transport to leaves    :    .6059E-07 volatilised : -.5781E-07 kg
 Transport to stem      :    .6314E-07 to fruits   :  .2378E-09 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :  .6507E-09 m/s
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OrgC=0.05: CSoil=5 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.5000E-05
.1000E+01	.8193E-06	.8734E-06	.3946E-06	.1797E-06	.5000E-05
.2000E+01	.8193E-06	.8789E-06	.3946E-06	.2518E-06	.5000E-05
.3000E+01	.8193E-06	.8830E-06	.3946E-06	.2712E-06	.5000E-05
.4000E+01	.8193E-06	.8863E-06	.3946E-06	.2689E-06	.5000E-05
.5000E+01	.8193E-06	.8889E-06	.3946E-06	.2574E-06	.5000E-05
.6000E+01	.8193E-06	.8911E-06	.3946E-06	.2425E-06	.5000E-05
.7000E+01	.8193E-06	.8929E-06	.3946E-06	.2268E-06	.5000E-05
.8000E+01	.8193E-06	.8944E-06	.3946E-06	.2116E-06	.5000E-05
.9000E+01	.8193E-06	.8957E-06	.3946E-06	.1974E-06	.5000E-05
.1000E+02	.8193E-06	.8968E-06	.3946E-06	.1845E-06	.5000E-05
.1100E+02	.8193E-06	.8978E-06	.3946E-06	.1727E-06	.5000E-05
.1200E+02	.8193E-06	.8987E-06	.3946E-06	.1621E-06	.5000E-05
.1300E+02	.8193E-06	.8995E-06	.3946E-06	.1525E-06	.5000E-05
.1400E+02	.8193E-06	.9002E-06	.3946E-06	.1439E-06	.5000E-05
.1500E+02	.8193E-06	.9009E-06	.3946E-06	.1361E-06	.5000E-05
.1600E+02	.8193E-06	.9014E-06	.3946E-06	.1291E-06	.5000E-05
.1700E+02	.8193E-06	.9020E-06	.3946E-06	.1227E-06	.5000E-05
.1800E+02	.8193E-06	.9024E-06	.3946E-06	.1169E-06	.5000E-05
.1900E+02	.8193E-06	.9029E-06	.3946E-06	.1115E-06	.5000E-05
.2000E+02	.8193E-06	.9033E-06	.3946E-06	.1067E-06	.5000E-05
.2100E+02	.8193E-06	.9036E-06	.3946E-06	.1022E-06	.5000E-05
.2200E+02	.8193E-06	.9040E-06	.3946E-06	.9812E-07	.5000E-05
.2300E+02	.8193E-06	.9043E-06	.3946E-06	.9432E-07	.5000E-05
.2400E+02	.8193E-06	.9046E-06	.3946E-06	.9080E-07	.5000E-05
.2500E+02	.8193E-06	.9049E-06	.3946E-06	.8754E-07	.5000E-05
.2600E+02	.8193E-06	.9051E-06	.3946E-06	.8450E-07	.5000E-05
.2700E+02	.8193E-06	.9054E-06	.3946E-06	.8166E-07	.5000E-05
.2800E+02	.8193E-06	.9056E-06	.3946E-06	.7901E-07	.5000E-05
.2900E+02	.8193E-06	.9058E-06	.3946E-06	.7652E-07	.5000E-05
.3000E+02	.8193E-06	.9060E-06	.3946E-06	.7418E-07	.5000E-05
.3100E+02	.8193E-06	.9062E-06	.3946E-06	.7198E-07	.5000E-05
.3200E+02	.8193E-06	.9064E-06	.3946E-06	.6991E-07	.5000E-05
.3300E+02	.8193E-06	.9066E-06	.3946E-06	.6796E-07	.5000E-05
.3400E+02	.8193E-06	.9068E-06	.3946E-06	.6611E-07	.5000E-05
.3500E+02	.8193E-06	.9069E-06	.3946E-06	.6436E-07	.5000E-05
.3600E+02	.8193E-06	.9071E-06	.3946E-06	.6269E-07	.5000E-05
.3700E+02	.8193E-06	.9072E-06	.3946E-06	.6112E-07	.5000E-05
.3800E+02	.8193E-06	.9073E-06	.3946E-06	.5962E-07	.5000E-05
.3900E+02	.8193E-06	.9075E-06	.3946E-06	.5819E-07	.5000E-05
.4000E+02	.8193E-06	.9076E-06	.3946E-06	.5683E-07	.5000E-05
.4100E+02	.8193E-06	.9077E-06	.3946E-06	.5553E-07	.5000E-05
.4200E+02	.8193E-06	.9078E-06	.3946E-06	.5429E-07	.5000E-05
.4300E+02	.8193E-06	.9079E-06	.3946E-06	.5310E-07	.5000E-05
.4400E+02	.8193E-06	.9080E-06	.3946E-06	.5196E-07	.5000E-05
.4500E+02	.8193E-06	.9081E-06	.3946E-06	.5087E-07	.5000E-05
.4600E+02	.8193E-06	.9082E-06	.3946E-06	.4983E-07	.5000E-05
.4700E+02	.8193E-06	.9083E-06	.3946E-06	.4883E-07	.5000E-05
.4800E+02	.8193E-06	.9084E-06	.3946E-06	.4787E-07	.5000E-05
.4900E+02	.8193E-06	.9085E-06	.3946E-06	.4694E-07	.5000E-05
.5000E+02	.8193E-06	.9086E-06	.3946E-06	.4605E-07	.5000E-05
.5100E+02	.8193E-06	.9087E-06	.3946E-06	.4519E-07	.5000E-05
.5200E+02	.8193E-06	.9087E-06	.3946E-06	.4437E-07	.5000E-05
.5300E+02	.8193E-06	.9088E-06	.3946E-06	.4357E-07	.5000E-05
.5400E+02	.8193E-06	.9089E-06	.3946E-06	.4280E-07	.5000E-05
.5500E+02	.8193E-06	.9090E-06	.3946E-06	.4206E-07	.5000E-05
.5600E+02	.8193E-06	.9090E-06	.3946E-06	.4135E-07	.5000E-05
.5700E+02	.8193E-06	.9091E-06	.3946E-06	.4065E-07	.5000E-05

.5800E+02	.8193E-06	.9092E-06	.3946E-06	.3998E-07	.5000E-05
.5900E+02	.8193E-06	.9092E-06	.3946E-06	.3934E-07	.5000E-05
.6000E+02	.8193E-06	.9093E-06	.3946E-06	.3871E-07	.5000E-05
.6100E+02	.8193E-06	.9093E-06	.3946E-06	.3810E-07	.5000E-05
.6200E+02	.8193E-06	.9094E-06	.3946E-06	.3751E-07	.5000E-05
.6300E+02	.8193E-06	.9095E-06	.3946E-06	.3694E-07	.5000E-05
.6400E+02	.8193E-06	.9095E-06	.3946E-06	.3639E-07	.5000E-05
.6500E+02	.8193E-06	.9096E-06	.3946E-06	.3585E-07	.5000E-05
.6600E+02	.8193E-06	.9096E-06	.3946E-06	.3533E-07	.5000E-05
.6700E+02	.8193E-06	.9097E-06	.3946E-06	.3482E-07	.5000E-05
.6800E+02	.8193E-06	.9097E-06	.3946E-06	.3433E-07	.5000E-05
.6900E+02	.8193E-06	.9098E-06	.3946E-06	.3385E-07	.5000E-05
.7000E+02	.8193E-06	.9098E-06	.3946E-06	.3339E-07	.5000E-05
.7100E+02	.8193E-06	.9098E-06	.3946E-06	.3294E-07	.5000E-05
.7200E+02	.8193E-06	.9099E-06	.3946E-06	.3249E-07	.5000E-05
.7300E+02	.8193E-06	.9099E-06	.3946E-06	.3207E-07	.5000E-05
.7400E+02	.8193E-06	.9100E-06	.3946E-06	.3165E-07	.5000E-05
.7500E+02	.8193E-06	.9100E-06	.3946E-06	.3124E-07	.5000E-05
.7600E+02	.8193E-06	.9100E-06	.3946E-06	.3084E-07	.5000E-05
.7700E+02	.8193E-06	.9101E-06	.3946E-06	.3046E-07	.5000E-05
.7800E+02	.8193E-06	.9101E-06	.3946E-06	.3008E-07	.5000E-05
.7900E+02	.8193E-06	.9102E-06	.3946E-06	.2971E-07	.5000E-05
.8000E+02	.8193E-06	.9102E-06	.3946E-06	.2935E-07	.5000E-05
.8100E+02	.8193E-06	.9102E-06	.3946E-06	.2900E-07	.5000E-05
.8200E+02	.8193E-06	.9103E-06	.3946E-06	.2866E-07	.5000E-05
.8300E+02	.8193E-06	.9103E-06	.3946E-06	.2833E-07	.5000E-05
.8400E+02	.8193E-06	.9103E-06	.3946E-06	.2800E-07	.5000E-05
.8500E+02	.8193E-06	.9103E-06	.3946E-06	.2768E-07	.5000E-05
.8600E+02	.8193E-06	.9104E-06	.3946E-06	.2737E-07	.5000E-05
.8700E+02	.8193E-06	.9104E-06	.3946E-06	.2706E-07	.5000E-05
.8800E+02	.8193E-06	.9104E-06	.3946E-06	.2676E-07	.5000E-05
.8900E+02	.8193E-06	.9105E-06	.3946E-06	.2647E-07	.5000E-05
.9000E+02	.8193E-06	.9105E-06	.3946E-06	.2619E-07	.5000E-05
.9100E+02	.8193E-06	.9105E-06	.3946E-06	.2591E-07	.5000E-05
.9200E+02	.8193E-06	.9105E-06	.3946E-06	.2563E-07	.5000E-05
.9300E+02	.8193E-06	.9106E-06	.3946E-06	.2537E-07	.5000E-05
.9400E+02	.8193E-06	.9106E-06	.3946E-06	.2510E-07	.5000E-05
.9500E+02	.8193E-06	.9106E-06	.3946E-06	.2485E-07	.5000E-05
.9600E+02	.8193E-06	.9106E-06	.3946E-06	.2460E-07	.5000E-05
.9700E+02	.8193E-06	.9107E-06	.3946E-06	.2435E-07	.5000E-05
.9800E+02	.8193E-06	.9107E-06	.3946E-06	.2411E-07	.5000E-05
.9900E+02	.8193E-06	.9107E-06	.3946E-06	.2387E-07	.5000E-05

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  Model PlantX by Stefan Trapp
OrgC=0.05; CSoil=27 ppb; CAir=30 ppt
  MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
  Equilibrium constants
   soil-water  :     .9287E+01
   air - soil  :     .4275E-01 air-water   :    .3970E+00
   root- soil  :     .1639E+00 root-water  :    .1522E+01
   leaves-soil :     .5621E+00 leaves-water:    .5221E+01
   TSCF        :     .7047E+00
 Simulation run time (days) :    .1000E+03
 Amount in Roots :   .5744E-08 Metabolites:   .1019E-06 kg
 Amount in Stems :   .6671E-09 Metabolites:   .1208E-07 kg
 Amount in Leaves:   .1427E-09 Metabolites:   .2599E-08 kg
 Amount in Fruits:   .3728E-10 Metabolites:   .1246E-08 kg
 Conc. in Root   :   .4424E-05 Metabolites:   .7852E-04 kg/m3
 Conc. in Stem   :   .4916E-05 Metabolites:   .8903E-04 kg/m3
 Conc. in leaf   :   .3952E-06 Metabolites:   .7199E-05 kg/m3
 Conc. in fruit  :   .1276E-06 Metabolites:   .4263E-05 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :   .1428E-06 with transp. stream
 Uptake with water diff.:  -.2465E-09 air diff.   : -.3493E-07 kg
 Transport to leaves    :   .3270E-06 volatilised : -.3242E-06 kg
 Transport to stem      :   .3409E-06 to fruits   :  .1283E-08 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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OrgC=0.05; CSoil=27 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.2700E-04
.1000E+01	.4424E-05	.4688E-05	.3952E-06	.9642E-06	.2700E-04
.2000E+01	.4424E-05	.4722E-05	.3952E-06	.1352E-05	.2700E-04
.3000E+01	.4424E-05	.4747E-05	.3952E-06	.1457E-05	.2700E-04
.4000E+01	.4424E-05	.4767E-05	.3952E-06	.1445E-05	.2700E-04
.5000E+01	.4424E-05	.4783E-05	.3952E-06	.1384E-05	.2700E-04
.6000E+01	.4424E-05	.4796E-05	.3952E-06	.1304E-05	.2700E-04
.7000E+01	.4424E-05	.4807E-05	.3952E-06	.1220E-05	.2700E-04
.8000E+01	.4424E-05	.4817E-05	.3952E-06	.1139E-05	.2700E-04
.9000E+01	.4424E-05	.4825E-05	.3952E-06	.1063E-05	.2700E-04
.1000E+02	.4424E-05	.4832E-05	.3952E-06	.9931E-06	.2700E-04
.1100E+02	.4424E-05	.4838E-05	.3952E-06	.9299E-06	.2700E-04
.1200E+02	.4424E-05	.4843E-05	.3952E-06	.8729E-06	.2700E-04
.1300E+02	.4424E-05	.4848E-05	.3952E-06	.8215E-06	.2700E-04
.1400E+02	.4424E-05	.4852E-05	.3952E-06	.7752E-06	.2700E-04
.1500E+02	.4424E-05	.4856E-05	.3952E-06	.7334E-06	.2700E-04
.1600E+02	.4424E-05	.4860E-05	.3952E-06	.6955E-06	.2700E-04
.1700E+02	.4424E-05	.4863E-05	.3952E-06	.6611E-06	.2700E-04
.1800E+02	.4424E-05	.4866E-05	.3952E-06	.6299E-06	.2700E-04
.1900E+02	.4424E-05	.4868E-05	.3952E-06	.6013E-06	.2700E-04
.2000E+02	.4424E-05	.4871E-05	.3952E-06	.5752E-06	.2700E-04
.2100E+02	.4424E-05	.4873E-05	.3952E-06	.5512E-06	.2700E-04
.2200E+02	.4424E-05	.4875E-05	.3952E-06	.5290E-06	.2700E-04
.2300E+02	.4424E-05	.4877E-05	.3952E-06	.5086E-06	.2700E-04
.2400E+02	.4424E-05	.4879E-05	.3952E-06	.4897E-06	.2700E-04
.2500E+02	.4424E-05	.4881E-05	.3952E-06	.4721E-06	.2700E-04
.2600E+02	.4424E-05	.4882E-05	.3952E-06	.4557E-06	.2700E-04
.2700E+02	.4424E-05	.4884E-05	.3952E-06	.4404E-06	.2700E-04
.2800E+02	.4424E-05	.4885E-05	.3952E-06	.4261E-06	.2700E-04
.2900E+02	.4424E-05	.4886E-05	.3952E-06	.4127E-06	.2700E-04
.3000E+02	.4424E-05	.4888E-05	.3952E-06	.4001E-06	.2700E-04
.3100E+02	.4424E-05	.4889E-05	.3952E-06	.3883E-06	.2700E-04
.3200E+02	.4424E-05	.4890E-05	.3952E-06	.3771E-06	.2700E-04
.3300E+02	.4424E-05	.4891E-05	.3952E-06	.3666E-06	.2700E-04
.3400E+02	.4424E-05	.4892E-05	.3952E-06	.3566E-06	.2700E-04
.3500E+02	.4424E-05	.4893E-05	.3952E-06	.3472E-06	.2700E-04
.3600E+02	.4424E-05	.4894E-05	.3952E-06	.3382E-06	.2700E-04
.3700E+02	.4424E-05	.4895E-05	.3952E-06	.3297E-06	.2700E-04
.3800E+02	.4424E-05	.4896E-05	.3952E-06	.3216E-06	.2700E-04
.3900E+02	.4424E-05	.4896E-05	.3952E-06	.3139E-06	.2700E-04
.4000E+02	.4424E-05	.4897E-05	.3952E-06	.3066E-06	.2700E-04
.4100E+02	.4424E-05	.4898E-05	.3952E-06	.2996E-06	.2700E-04
.4200E+02	.4424E-05	4899E-05	.3952E-06	.2929E-06	.2700E-04
.4300E+02	.4424E-05	.4899E-05	.3952E-06	.2865E-06	.2700E-04
.4400E+02	.4424E-05	.4900E-05	.3952E-06	.2804E-06	.2700E-04
.4500E+02	.4424E-05	.4900E-05	.3952E-06	.2745E-06	.2700E-04
.4600E+02	.4424E-05	.4901E-05	.3952E-06	.2689E-06	.2700E-04
.4700E+02	.4424E-05	.4902E-05	.3952E-06	.2635E-06	.2700E-04
.4800E+02	.4424E-05	.4902E-05	.3952E-06	.2583E-06	.2700E-04
.4900E+02	.4424E-05	.4903E-05	.3952E-06	.2533E-06	.2700E-04
.5000E+02	.4424E-05	.4903E-05	.3952E-06	.2485E-06	.2700E-04
.5100E+02	.4424E-05	.4904E-05	.3952E-06	.2439E-06	.2700E-04
.5200E+02	.4424E-05	.4904E-05	.3952E-06	.2394E-06	.2700E-04
.5300E+02	.4424E-05	.4905E-05	.3952E-06	.2351E-06	.2700E-04
.5400E+02	.4424E-05	.4905E-05	.3952E-06	.2310E-06	.2700E-04
.5500E+02	.4424E-05	.4906E-05	.3952E-06	.2270E-06	.2700E-04
.5600E+02	.4424E-05	.4906E-05	.3952E-06	.2231E-06	.2700E-04
.5700E+02	.4424E-05	.4906E-05	.3952E-06	.2194E-06	.2700E-04

.5800E+02	.4424E-05	.4907E-05	.3952E-06	.2158E-06	.2700E-04
.5900E+02	.4424E-05	.4907E-05	.3952E-06	.2123E-06	.2700E-04
.6000E+02	.4424E-05	.4907E-05	.3952E-06	.2089E-06	.2700E-04
.6100E+02	.4424E-05	.4908E-05	.3952E-06	.2056E-06	.2700E-04
.6200E+02	.4424E-05	.4908E-05	.3952E-06	.2025E-06	.2700E-04
.6300E+02	.4424E-05	.4909E-05	.3952E-06	.1994E-06	.2700E-04
.6400E+02	.4424E-05	.4909E-05	.3952E-06	.1964E-06	.2700E-04
.6500E+02	.4424E-05	.4909E-05	.3952E-06	.1935E-06	.2700E-04
.6600E+02	.4424E-05	.4909E-05	.3952E-06	.1907E-06	.2700E-04
.6700E+02	.4424E-05	.4910E-05	.3952E-06	.1880E-06	.2700E-04
.6800E+02	.4424E-05	.4910E-05	.3952E-06	.1853E-06	.2700E-04
.6900E+02	.4424E-05	.4910E-05	.3952E-06	.1827E-06	.2700E-04
.7000E+02	.4424E-05	.4911E-05	.3952E-06	.1802E-06	.2700E-04
.7100E+02	.4424E-05	.4911E-05	.3952E-06	.1778E-06	.2700E-04
.7200E+02	.4424E-05	.4911E-05	.3952E-06	.1754E-06	.2700E-04
.7300E+02	.4424E-05	.4911E-05	.3952E-06	.1731E-06	.2700E-04
.7400E+02	.4424E-05	.4912E-05	.3952E-06	.1708E-06	.2700E-04
.7500E+02	.4424E-05	.4912E-05	.3952E-06	.1686E-06	.2700E-04
.7600E+02	.4424E-05	.4912E-05	.3952E-06	.1665E-06	.2700E-04
.7700E+02	.4424E-05	.4912E-05	.3952E-06	.1644E-06	.2700E-04
.7800E+02	.4424E-05	.4913E-05	.3952E-06	.1624E-06	.2700E-04
.7900E+02	.4424E-05	.4913E-05	.3952E-06	.1604E-06	.2700E-04
.8000E+02	.4424E-05	.4913E-05	.3952E-06	.1584E-06	.2700E-04
.8100E+02	.4424E-05	.4913E-05	.3952E-06	.1565E-06	.2700E-04
.8200E+02	.4424E-05	.4913E-05	.3952E-06	.1547E-06	.2700E-04
.8300E+02	.4424E-05	.4914E-05	.3952E-06	.1529E-06	.2700E-04
.8400E+02	.4424E-05	.4914E-05	.3952E-06	.1511E-06	.2700E-04
.8500E+02	.4424E-05	.4914E-05	.3952E-06	.1494E-06	.2700E-04
.8600E+02	.4424E-05	.4914E-05	.3952E-06	.1477E-06	.2700E-04
.8700E+02	.4424E-0				

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Not ready error reading file
B:\PLANTX\PLOT

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  Model PlantX by Stefan Trapp
OrgC=0.05; CSoil=30 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:    .2290E+01 Henry:    .3970E+00 Halftime:    .2300E+01
  Equilibrium constants
   soil-water  :      .9287E+01
   air - soil  :      .4275E-01 air-water    :     .3970E+00
   root- soil  :      .1639E+00 root-water   :     .1522E+01
   leaves-soil :      .5621E+00 leaves-water:      .5221E+01
   TSCF        :      .7047E+00
 Simulation run time (days) :      .1000E+03
 Amount in Roots :    .6382E-08 Metabolites:    .1133E-06 kg
 Amount in Stems :    .7413E-09 Metabolites:    .1342E-07 kg
 Amount in Leaves:    .1427E-09 Metabolites:    .2600E-08 kg
 Amount in Fruits:    .4143E-10 Metabolites:    .1384E-08 kg
 Conc. in Root   :    .4916E-05 Metabolites:    .8725E-04 kg/m3
 Conc. in Stem   :    .5462E-05 Metabolites:    .9892E-04 kg/m3
 Conc. in leaf   :    .3953E-06 Metabolites:    .7200E-05 kg/m3
 Conc. in fruit  :    .1418E-06 Metabolites:    .4737E-05 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :    .1587E-06 with transp. stream
 Uptake with water diff.:   -.2739E-09 air diff.    : -.3882E-07 kg
 Transport to leaves    :    .3633E-06 volatilised : -.3605E-06 kg
 Transport to stem      :    .3788E-06 to fruits    :  .1425E-08 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :  .6507E-09 m/s
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OrgC=0.05; CSoil=30 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.3000E-04
.1000E+01	.4916E-05	.5208E-05	.3952E-06	.1071E-05	.3000E-04
.2000E+01	.4916E-05	.5246E-05	.3952E-06	.1502E-05	.3000E-04
.3000E+01	.4916E-05	.5274E-05	.3952E-06	.1619E-05	.3000E-04
.4000E+01	.4916E-05	.5296E-05	.3952E-06	.1605E-05	.3000E-04
.5000E+01	.4916E-05	.5314E-05	.3952E-06	.1537E-05	.3000E-04
.6000E+01	.4916E-05	.5329E-05	.3952E-06	.1449E-05	.3000E-04
.7000E+01	.4916E-05	.5341E-05	.3952E-06	.1356E-05	.3000E-04
.8000E+01	.4916E-05	.5351E-05	.3952E-06	.1265E-05	.3000E-04
.9000E+01	.4916E-05	.5360E-05	.3952E-06	.1181E-05	.3000E-04
.1000E+02	.4916E-05	.5368E-05	.3952E-06	.1103E-05	.3000E-04
.1100E+02	.4916E-05	.5375E-05	.3952E-06	.1033E-05	.3000E-04
.1200E+02	.4916E-05	.5381E-05	.3952E-06	.9699E-06	.3000E-04
.1300E+02	.4916E-05	.5386E-05	.3952E-06	.9128E-06	.3000E-04
.1400E+02	.4916E-05	.5391E-05	.3952E-06	.8613E-06	.3000E-04
.1500E+02	.4916E-05	.5395E-05	.3952E-06	.8148E-06	.3000E-04
.1600E+02	.4916E-05	.5399E-05	.3952E-06	.7727E-06	.3000E-04
.1700E+02	.4916E-05	.5403E-05	.3952E-06	.7346E-06	.3000E-04
.1800E+02	.4916E-05	.5406E-05	.3952E-06	.6998E-06	.3000E-04
.1900E+02	.4916E-05	.5409E-05	.3952E-06	.6681E-06	.3000E-04
.2000E+02	.4916E-05	.5412E-05	.3952E-06	.6391E-06	.3000E-04
.2100E+02	.4916E-05	.5414E-05	.3952E-06	.6124E-06	.3000E-04
.2200E+02	.4916E-05	.5417E-05	.3952E-06	.5878E-06	.3000E-04
.2300E+02	.4916E-05	.5419E-05	.3952E-06	.5651E-06	.3000E-04
.2400E+02	.4916E-05	.5421E-05	.3952E-06	.5441E-06	.3000E-04
.2500E+02	.4916E-05	.5423E-05	.3953E-06	.5245E-06	.3000E-04
.2600E+02	.4916E-05	.5425E-05	.3953E-06	.5063E-06	.3000E-04
.2700E+02	.4916E-05	.5426E-05	.3953E-06	.4893E-06	.3000E-04
.2800E+02	.4916E-05	.5428E-05	.3953E-06	.4735E-06	.3000E-04
.2900E+02	.4916E-05	.5429E-05	.3953E-06	.4586E-06	.3000E-04
.3000E+02	.4916E-05	.5431E-05	.3953E-06	.4446E-06	.3000E-04
.3100E+02	.4916E-05	.5432E-05	.3953E-06	.4314E-06	.3000E-04
.3200E+02	.4916E-05	.5433E-05	.3953E-06	.4190E-06	.3000E-04
.3300E+02	.4916E-05	.5434E-05	.3953E-06	.4073E-06	.3000E-04
.3400E+02	.4916E-05	.5436E-05	.3953E-06	.3962E-06	.3000E-04
.3500E+02	.4916E-05	.5437E-05	.3953E-06	.3858E-06	.3000E-04
.3600E+02	.4916E-05	.5438E-05	.3953E-06	.3758E-06	.3000E-04
.3700E+02	.4916E-05	.5439E-05	.3953E-06	.3664E-06	.3000E-04
.3800E+02	.4916E-05	.5439E-05	.3953E-06	.3574E-06	.3000E-04
.3900E+02	.4916E-05	.5440E-05	.3953E-06	.3488E-06	.3000E-04
.4000E+02	.4916E-05	.5441E-05	.3953E-06	.3407E-06	.3000E-04
.4100E+02	.4916E-05	.5442E-05	.3953E-06	.3329E-06	.3000E-04
.4200E+02	.4916E-05	.5443E-05	.3953E-06	.3254E-06	.3000E-04
.4300E+02	.4916E-05	.5444E-05	.3953E-06	.3183E-06	.3000E-04
.4400E+02	.4916E-05	.5444E-05	.3953E-06	.3115E-06	.3000E-04
.4500E+02	.4916E-05	.5445E-05	.3953E-06	.3050E-06	.3000E-04
.4600E+02	.4916E-05	.5446E-05	.3953E-06	.2988E-06	.3000E-04
.4700E+02	.4916E-05	.5446E-05	.3953E-06	.2928E-06	.3000E-04
.4800E+02	.4916E-05	.5447E-05	.3953E-06	.2870E-06	.3000E-04
.4900E+02	.4916E-05	.5447E-05	.3953E-06	.2814E-06	.3000E-04
.5000E+02	.4916E-05	.5448E-05	.3953E-06	.2761E-06	.3000E-04
.5100E+02	.4916E-05	.5448E-05	.3953E-06	.2710E-06	.3000E-04
.5200E+02	.4916E-05	.5449E-05	.3953E-06	.2660E-06	.3000E-04
.5300E+02	.4916E-05	.5450E-05	.3953E-06	.2613E-06	.3000E-04
.5400E+02	.4916E-05	.5450E-05	.3953E-06	.2567E-06	.3000E-04
.5500E+02	.4916E-05	.5450E-05	.3953E-06	.2522E-06	.3000E-04
.5600E+02	.4916E-05	.5451E-05	.3953E-06	.2479E-06	.3000E-04
.5700E+02	.4916E-05	.5451E-05	.3953E-06	.2438E-06	.3000E-04

.5800E+02	.4916E-05	.5452E-05	.3953E-06	.2398E-06	.3000E-04
.5900E+02	.4916E-05	.5452E-05	.3953E-06	.2359E-06	.3000E-04
.6000E+02	.4916E-05	.5453E-05	.3953E-06	.2321E-06	.3000E-04
.6100E+02	.4916E-05	.5453E-05	.3953E-06	.2285E-06	.3000E-04
.6200E+02	.4916E-05	.5453E-05	.3953E-06	.2250E-06	.3000E-04
.6300E+02	.4916E-05	.5454E-05	.3953E-06	.2215E-06	.3000E-04
.6400E+02	.4916E-05	.5454E-05	.3953E-06	.2182E-06	.3000E-04
.6500E+02	.4916E-05	.5455E-05	.3953E-06	.2150E-06	.3000E-04
.6600E+02	.4916E-05	.5455E-05	.3953E-06	.2119E-06	.3000E-04
.6700E+02	.4916E-05	.5455E-05	.3953E-06	.2088E-06	.3000E-04
.6800E+02	.4916E-05	.5456E-05	.3953E-06	.2059E-06	.3000E-04
.6900E+02	.4916E-05	.5456E-05	.3953E-06	.2030E-06	.3000E-04
.7000E+02	.4916E-05	.5456E-05	.3953E-06	.2002E-06	.3000E-04
.7100E+02	.4916E-05	.5456E-05	.3953E-06	.1975E-06	.3000E-04
.7200E+02	.4916E-05	.5457E-05	.3953E-06	.1949E-06	.3000E-04
.7300E+02	.4916E-05	.5457E-05	.3953E-06	.1923E-06	.3000E-04
.7400E+02	.4916E-05	.5457E-05	.3953E-06	.1898E-06	.3000E-04
.7500E+02	.4916E-05	.5458E-05	.3953E-06	.1874E-06	.3000E-04
.7600E+02	.4916E-05	.5458E-05	.3953E-06	.1850E-06	.3000E-04
.7700E+02	.4916E-05	.5458E-05	.3953E-06	.1827E-06	.3000E-04
.7800E+02	.4916E-05	.5458E-05	.3953E-06	.1804E-06	.3000E-04
.7900E+02	.4916E-05	.5459E-05	.3953E-06	.1782E-06	.3000E-04
.8000E+02	.4916E-05	.5459E-05	.3953E-06	.1760E-06	.3000E-04
.8100E+02	.4916E-05	.5459E-05	.3953E-06	.1739E-06	.3000E-04
.8200E+02	.4916E-05	.5459E-05	.3953E-06	.1719E-06	.3000E-04
.8300E+02	.4916E-05	.5459E-05	.3953E-06	.1699E-06	.3000E-04
.8400E+02	.4916E-05	.5460E-05	.3953E-06	.1679E-06	.3000E-04
.8500E+02	.4916E-05	.5460E-05	.3953E-06	.1660E-06	.3000E-04
.8600E+02	.4916E-05	.5460E-05	.3953E-06	.1641E-06	.3000E-04
.8700E+02	.4916E-05	.5460E-05	.3953E-06	.1623E-06	.3000E-04
.8800E+02	.4916E-05	.5460E-05	.3953E-06	.1605E-06	.3000E-04
.8900E+02	.4916E-05	.5461E-05	.3953E-06	.1588E-06	.3000E-04
.9000E+02	.4916E-05	.5461E-05	.3953E-06	.1571E-06	.3000E-04
.9100E+02	.4916E-05	.5461E-05	.3953E-06	.1554E-06	.3000E-04
.9200E+02	.4916E-05	.5461E-05	.3953E-06	.1537E-06	.3000E-04
.9300E+02	.4916E-05	.5461E-05	.3953E-06	.1521E-06	.3000E-04
.9400E+02	.4916E-05	.5462E-05	.3953E-06	.1506E-06	.3000E-04
.9500E+02	.4916E-05	.5462E-05	.3953E-06	.1490E-06	.3000E-04
.9600E+02	.4916E-05	.5462E-05	.3953E-06	.1475E-06	.3000E-04
.9700E+02	.4916E-05	.5462E-05	.3953E-06	.1460E-06	.3000E-04
.9800E+02	.4916E-05	.5462E-05	.3953E-06	.1446E-06	.3000E-04
.9900E+02	.4916E-05	.5462E-05	.3953E-06	.1432E-06	.3000E-04

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  Model PlantX by Stefan Trapp
OrgC=0.05; CSoil=1057 ppb; CAir=30 ppt
  MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
  Equilibrium constants
   soil-water  :      .9287E+01
   air - soil  :      .4275E-01 air-water    :     .3970E+00
   root- soil  :      .1639E+00 root-water   :     .1522E+01
   leaves-soil :      .5621E+00 leaves-water:      .5221E+01
   TSCF        :      .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :    .2249E-06 Metabolites:    .3991E-05 kg
 Amount in Stems :    .2612E-07 Metabolites:    .4729E-06 kg
 Amount in Leaves:    .1518E-09 Metabolites:    .2765E-08 kg
 Amount in Fruits:    .1459E-08 Metabolites:    .4875E-07 kg
 Conc. in Root   :    .1732E-03 Metabolites:    .3074E-02 kg/m3
 Conc. in Stem   :    .1924E-03 Metabolites:    .3485E-02 kg/m3
 Conc. in leaf   :    .4205E-06 Metabolites:    .7656E-05 kg/m3
 Conc. in fruit  :    .4995E-05 Metabolites:    .1669E-03 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :   .5592E-05 with transp. stream
 Uptake with water diff.:  -.9651E-08 air diff.    : -.1368E-05 kg
 Transport to leaves    :   .1280E-04 volatilised : -.1279E-04 kg
 Transport to stem      :   .1335E-04 to fruits    :  .5021E-07 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :   .6507E-09 m/s
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OrgC=0.05; CSoil=1057 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.1057E-02
.1000E+01	.1732E-03	.1833E-03	.4192E-06	.3769E-04	.1057E-02
.2000E+01	.1732E-03	.1846E-03	.4194E-06	.5285E-04	.1057E-02
.3000E+01	.1732E-03	.1857E-03	.4195E-06	.5697E-04	.1057E-02
.4000E+01	.1732E-03	.1865E-03	.4196E-06	.5650E-04	.1057E-02
.5000E+01	.1732E-03	.1871E-03	.4197E-06	.5411E-04	.1057E-02
.6000E+01	.1732E-03	.1876E-03	.4198E-06	.5100E-04	.1057E-02
.7000E+01	.1732E-03	.1881E-03	.4199E-06	.4773E-04	.1057E-02
.8000E+01	.1732E-03	.1884E-03	.4199E-06	.4455E-04	.1057E-02
.9000E+01	.1732E-03	.1888E-03	.4200E-06	.4158E-04	.1057E-02
.1000E+02	.1732E-03	.1890E-03	.4200E-06	.3885E-04	.1057E-02
.1100E+02	.1732E-03	.1893E-03	.4200E-06	.3638E-04	.1057E-02
.1200E+02	.1732E-03	.1895E-03	.4201E-06	.3415E-04	.1057E-02
.1300E+02	.1732E-03	.1897E-03	.4201E-06	.3214E-04	.1057E-02
.1400E+02	.1732E-03	.1899E-03	.4201E-06	.3033E-04	.1057E-02
.1500E+02	.1732E-03	.1900E-03	.4201E-06	.2870E-04	.1057E-02
.1600E+02	.1732E-03	.1902E-03	.4201E-06	.2722E-04	.1057E-02
.1700E+02	.1732E-03	.1903E-03	.4202E-06	.2587E-04	.1057E-02
.1800E+02	.1732E-03	.1904E-03	.4202E-06	.2465E-04	.1057E-02
.1900E+02	.1732E-03	.1905E-03	.4202E-06	.2353E-04	.1057E-02
.2000E+02	.1732E-03	.1906E-03	.4202E-06	.2251E-04	.1057E-02
.2100E+02	.1732E-03	.1907E-03	.4202E-06	.2157E-04	.1057E-02
.2200E+02	.1732E-03	.1908E-03	.4202E-06	.2070E-04	.1057E-02
.2300E+02	.1732E-03	.1909E-03	.4202E-06	.1990E-04	.1057E-02
.2400E+02	.1732E-03	.1910E-03	.4202E-06	.1916E-04	.1057E-02
.2500E+02	.1732E-03	.1910E-03	.4203E-06	.1848E-04	.1057E-02
.2600E+02	.1732E-03	.1911E-03	.4203E-06	.1784E-04	.1057E-02
.2700E+02	.1732E-03	.1911E-03	.4203E-06	.1724E-04	.1057E-02
.2800E+02	.1732E-03	.1912E-03	.4203E-06	.1668E-04	.1057E-02
.2900E+02	.1732E-03	.1913E-03	.4203E-06	.1615E-04	.1057E-02
.3000E+02	.1732E-03	.1913E-03	.4203E-06	.1566E-04	.1057E-02
.3100E+02	.1732E-03	.1913E-03	.4203E-06	.1520E-04	.1057E-02
.3200E+02	.1732E-03	.1914E-03	.4203E-06	.1476E-04	.1057E-02
.3300E+02	.1732E-03	.1914E-03	.4203E-06	.1435E-04	.1057E-02
.3400E+02	.1732E-03	.1915E-03	.4203E-06	.1396E-04	.1057E-02
.3500E+02	.1732E-03	.1915E-03	.4203E-06	.1359E-04	.1057E-02
.3600E+02	.1732E-03	.1916E-03	.4203E-06	.1324E-04	.1057E-02
.3700E+02	.1732E-03	.1916E-03	.4203E-06	.1291E-04	.1057E-02
.3800E+02	.1732E-03	.1916E-03	.4203E-06	.1259E-04	.1057E-02
.3900E+02	.1732E-03	.1917E-03	.4203E-06	.1229E-04	.1057E-02
.4000E+02	.1732E-03	.1917E-03	.4203E-06	.1200E-04	.1057E-02
.4100E+02	.1732E-03	.1917E-03	.4204E-06	.1173E-04	.1057E-02
.4200E+02	.1732E-03	.1917E-03	.4204E-06	.1146E-04	.1057E-02
.4300E+02	.1732E-03	.1918E-03	.4204E-06	.1121E-04	.1057E-02
.4400E+02	.1732E-03	.1918E-03	.4204E-06	.1097E-04	.1057E-02
.4500E+02	.1732E-03	.1918E-03	.4204E-06	.1074E-04	.1057E-02
.4600E+02	.1732E-03	.1918E-03	.4204E-06	.1052E-04	.1057E-02
.4700E+02	.1732E-03	.1919E-03	.4204E-06	.1031E-04	.1057E-02
.4800E+02	.1732E-03	.1919E-03	.4204E-06	.1011E-04	.1057E-02
.4900E+02	.1732E-03	.1919E-03	.4204E-06	.9915E-05	.1057E-02
.5000E+02	.1732E-03	.1919E-03	.4204E-06	.9727E-05	.1057E-02
.5100E+02	.1732E-03	.1919E-03	.4204E-06	.9546E-05	.1057E-02
.5200E+02	.1732E-03	.1920E-03	.4204E-06	.9372E-05	.1057E-02
.5300E+02	.1732E-03	.1920E-03	.4204E-06	.9204E-05	.1057E-02
.5400E+02	.1732E-03	.1920E-03	.4204E-06	.9042E-05	.1057E-02
.5500E+02	.1732E-03	.1920E-03	.4204E-06	.8885E-05	.1057E-02
.5600E+02	.1732E-03	.1920E-03	.4204E-06	.8734E-05	.1057E-02
.5700E+02	.1732E-03	.1920E-03	.4204E-06	.8588E-05	.1057E-02

.5800E+02	.1732E-03	.1921E-03	.4204E-06	.8447E-05	.1057E-02
.5900E+02	.1732E-03	.1921E-03	.4204E-06	.8310E-05	.1057E-02
.6000E+02	.1732E-03	.1921E-03	.4204E-06	.8178E-05	.1057E-02
.6100E+02	.1732E-03	.1921E-03	.4204E-06	.8049E-05	.1057E-02
.6200E+02	.1732E-03	.1921E-03	.4204E-06	.7925E-05	.1057E-02
.6300E+02	.1732E-03	.1921E-03	.4204E-06	.7805E-05	.1057E-02
.6400E+02	.1732E-03	.1921E-03	.4204E-06	.7688E-05	.1057E-02
.6500E+02	.1732E-03	.1922E-03	.4204E-06	.7574E-05	.1057E-02
.6600E+02	.1732E-03	.1922E-03	.4204E-06	.7464E-05	.1057E-02
.6700E+02	.1732E-03	.1922E-03	.4204E-06	.7357E-05	.1057E-02
.6800E+02	.1732E-03	.1922E-03	.4204E-06	.7253E-05	.1057E-02
.6900E+02	.1732E-03	.1922E-03	.4204E-06	.7152E-05	.1057E-02
.7000E+02	.1732E-03	.1922E-03	.4204E-06	.7054E-05	.1057E-02
.7100E+02	.1732E-03	.1922E-03	.4204E-06	.6958E-05	.1057E-02
.7200E+02	.1732E-03	.1922E-03	.4204E-06	.6865E-05	.1057E-02
.7300E+02	.1732E-03	.1923E-03	.4204E-06	.6775E-05	.1057E-02
.7400E+02	.1732E-03	.1923E-03	.4204E-06	.6686E-05	.1057E-02
.7500E+02	.1732E-03	.1923E-03	.4204E-06	.6601E-05	.1057E-02
.7600E+02	.1732E-03	.1923E-03	.4204E-06	.6517E-05	.1057E-02
.7700E+02	.1732E-03	.1923E-03	.4204E-06	.6435E-05	.1057E-02
.7800E+02	.1732E-03	.1923E-03	.4204E-06	.6355E-05	.1057E-02
.7900E+02	.1732E-03	.1923E-03	.4204E-06	.6278E-05	.1057E-02
.8000E+02	.1732E-03	.1923E-03	.4204E-06	.6202E-05	.1057E-02
.8100E+02	.1732E-03	.1923E-03	.4204E-06	.6128E-05	.1057E-02
.8200E+02	.1732E-03	.1923E-03	.4204E-06	.6055E-05	.1057E-02
.8300E+02	.1732E-03	.1923E-03	.4204E-06	.5985E-05	.1057E-02
.8400E+02	.1732E-03	.1923E-03	.4204E-06	.5916E-05	.1057E-02
.8500E+02	.1732E-03	.1924E-03	.4204E-06	.5849E-05	.1057E-02
.8600E+02	.1732E-03	.1924E-03	.4204E-06	.5783E-05	.1057E-02
.8700E+02	.1732E-03	.1924E-03	.4204E-06	.5718E-05	.1057E-02
.8800E+02	.1732E-03	.1924E-03	.4204E-06	.5655E-05	.1057E-02
.8900E+02	.1732E-03	.1924E-03	.4204E-06	.5594E-05	.1057E-02
.9000E+02	.1732E-03	.1924E-03	.4204E-06	.5533E-05	.1057E-02
.9100E+02	.1732E-03	.1924E-03	.4204E-06	.5474E-05	.1057E-02
.9200E+02	.1732E-03	.1924E-03	.4204E-06	.5417E-05	.1057E-02
.9300E+02	.1732E-03	.1924E-03	.4204E-06	.5360E-05	.1057E-02
.9400E+02	.1732E-03	.1924E-03	.4204E-06	.5305E-05	.1057E-02
.9500E+02	.1732E-03	.1924E-03	.4204E-06	.5250E-05	.1057E-02
.9600E+02	.1732E-03	.1924E-03	.4204E-06	.5197E-05	.1057E-02
.9700E+02	.1732E-03	.1924E-03	.4204E-06	.5145E-05	.1057E-02
.9800E+02	.1732E-03	.1924E-03	.4204E-06	.5094E-05	.1057E-02
.9900E+02	.1732E-03	.1924E-03	.4205E-06	.5044E-05	.1057E-02

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 Model PlantX by Stefan Trapp
OrgC=0.05; CSoil=187710 ppb; CAir=30 ppt
 MW:    .1314E+03 logKow:    .2290E+01 Henry:    .3970E+00 Halftime:    .2000E+01
 Equilibrium constants
  soil-water   :      .9287E+01
  air - soil   :      .4275E-01 air-water    :      .3970E+00
  root- soil   :      .1639E+00 root-water   :      .1522E+01
  leaves-soil  :      .5621E+00 leaves-water:       .5221E+01
  TSCF         :      .7047E+00
Simulation run time (days) :    .1000E+03
Amount in Roots :   .3993E-04 Metabolites:   .7088E-03 kg
Amount in Stems :   .4638E-05 Metabolites:   .8398E-04 kg
Amount in Leaves:   .1805E-08 Metabolites:   .3271E-07 kg
Amount in Fruits:   .2592E-06 Metabolites:   .8658E-05 kg
Conc. in Root   :   .3076E-01 Metabolites:   .5459E+00 kg/m3
Conc. in Stem   :   .3418E-01 Metabolites:   .6189E+00 kg/m3
Conc. in leaf   :   .5000E-05 Metabolites:   .9058E-04 kg/m3
Conc. in fruit  :   .8870E-03 Metabolites:   .2963E-01 kg/m3
Total Transpiration m3 :    .1664E+00 phloem flux :   .6560E-03 m3
Uptake into roots      :    .9931E-03 with transp. stream
Uptake with water diff.:   -.1714E-05 air diff.    : -.2429E-03 kg
Transport to leaves    :    .2273E-02 volatilised : -.2273E-02 kg
Transport to stem      :    .2370E-02 to fruits    :  .8917E-05 kg
Conductivity of Stomata:    .8544E-03 of Cuticula :   .6507E-09 m/s
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OrgC=0.05; CSoil=187710 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.1877E+00
.1000E+01	.3076E-01	.3255E-01	.4780E-05	.6694E-02	.1877E+00
.2000E+01	.3076E-01	.3279E-01	.4813E-05	.9385E-02	.1877E+00
.3000E+01	.3076E-01	.3297E-01	.4837E-05	.1012E-01	.1877E+00
.4000E+01	.3076E-01	.3311E-01	.4856E-05	.1003E-01	.1877E+00
.5000E+01	.3076E-01	.3323E-01	.4872E-05	.9609E-02	.1877E+00
.6000E+01	.3076E-01	.3332E-01	.4884E-05	.9057E-02	.1877E+00
.7000E+01	.3076E-01	.3340E-01	.4895E-05	.8475E-02	.1877E+00
.8000E+01	.3076E-01	.3347E-01	.4904E-05	.7911E-02	.1877E+00
.9000E+01	.3076E-01	.3352E-01	.4911E-05	.7383E-02	.1877E+00
.1000E+02	.3076E-01	.3357E-01	.4918E-05	.6900E-02	.1877E+00
.1100E+02	.3076E-01	.3362E-01	.4924E-05	.6461E-02	.1877E+00
.1200E+02	.3076E-01	.3365E-01	.4929E-05	.6065E-02	.1877E+00
.1300E+02	.3076E-01	.3369E-01	.4934E-05	.5708E-02	.1877E+00
.1400E+02	.3076E-01	.3372E-01	.4938E-05	.5387E-02	.1877E+00
.1500E+02	.3076E-01	.3375E-01	.4942E-05	.5096E-02	.1877E+00
.1600E+02	.3076E-01	.3377E-01	.4945E-05	.4833E-02	.1877E+00
.1700E+02	.3076E-01	.3379E-01	.4948E-05	.4594E-02	.1877E+00
.1800E+02	.3076E-01	.3382E-01	.4951E-05	.4377E-02	.1877E+00
.1900E+02	.3076E-01	.3383E-01	.4954E-05	.4179E-02	.1877E+00
.2000E+02	.3076E-01	.3385E-01	.4956E-05	.3997E-02	.1877E+00
.2100E+02	.3076E-01	.3387E-01	.4958E-05	.3831E-02	.1877E+00
.2200E+02	.3076E-01	.3388E-01	.4960E-05	.3677E-02	.1877E+00
.2300E+02	.3076E-01	.3390E-01	.4962E-05	.3535E-02	.1877E+00
.2400E+02	.3076E-01	.3391E-01	.4964E-05	.3403E-02	.1877E+00
.2500E+02	.3076E-01	.3392E-01	.4965E-05	.3281E-02	.1877E+00
.2600E+02	.3076E-01	.3393E-01	.4967E-05	.3167E-02	.1877E+00
.2700E+02	.3076E-01	.3394E-01	.4968E-05	.3061E-02	.1877E+00
.2800E+02	.3076E-01	.3395E-01	.4970E-05	.2962E-02	.1877E+00
.2900E+02	.3076E-01	.3396E-01	.4971E-05	.2869E-02	.1877E+00
.3000E+02	.3076E-01	.3397E-01	.4972E-05	.2781E-02	.1877E+00
.3100E+02	.3076E-01	.3398E-01	.4973E-05	.2699E-02	.1877E+00
.3200E+02	.3076E-01	.3399E-01	.4974E-05	.2621E-02	.1877E+00
.3300E+02	.3076E-01	.3400E-01	.4975E-05	.2548E-02	.1877E+00
.3400E+02	.3076E-01	.3400E-01	.4976E-05	.2479E-02	.1877E+00
.3500E+02	.3076E-01	.3401E-01	.4977E-05	.2413E-02	.1877E+00
.3600E+02	.3076E-01	.3402E-01	.4978E-05	.2351E-02	.1877E+00
.3700E+02	.3076E-01	.3402E-01	.4979E-05	.2292E-02	.1877E+00
.3800E+02	.3076E-01	.3403E-01	.4980E-05	.2236E-02	.1877E+00
.3900E+02	.3076E-01	.3403E-01	.4981E-05	.2182E-02	.1877E+00
.4000E+02	.3076E-01	.3404E-01	.4981E-05	.2131E-02	.1877E+00
.4100E+02	.3076E-01	.3405E-01	.4982E-05	.2082E-02	.1877E+00
.4200E+02	.3076E-01	.3405E-01	.4983E-05	.2036E-02	.1877E+00
.4300E+02	.3076E-01	.3405E-01	.4983E-05	.1992E-02	.1877E+00
.4400E+02	.3076E-01	.3406E-01	.4984E-05	.1949E-02	.1877E+00
.4500E+02	.3076E-01	.3406E-01	.4984E-05	.1908E-02	.1877E+00
.4600E+02	.3076E-01	.3407E-01	.4985E-05	.1869E-02	.1877E+00
.4700E+02	.3076E-01	.3407E-01	.4986E-05	.1831E-02	.1877E+00
.4800E+02	.3076E-01	.3408E-01	.4986E-05	.1795E-02	.1877E+00
.4900E+02	.3076E-01	.3408E-01	.4987E-05	.1761E-02	.1877E+00
.5000E+02	.3076E-01	.3408E-01	.4987E-05	.1727E-02	.1877E+00
.5100E+02	.3076E-01	.3409E-01	.4988E-05	.1695E-02	.1877E+00
.5200E+02	.3076E-01	.3409E-01	.4988E-05	.1664E-02	.1877E+00
.5300E+02	.3076E-01	.3409E-01	.4988E-05	.1634E-02	.1877E+00
.5400E+02	.3076E-01	.3410E-01	.4989E-05	.1606E-02	.1877E+00
.5500E+02	.3076E-01	.3410E-01	.4989E-05	.1578E-02	.1877E+00
.5600E+02	.3076E-01	.3410E-01	.4990E-05	.1551E-02	.1877E+00
.5700E+02	.3076E-01	.3411E-01	.4990E-05	.1525E-02	.1877E+00

.5800E+02	.3076E-01	.3411E-01	.4990E-05	.1500E-02	.1877E+00
.5900E+02	.3076E-01	.3411E-01	.4991E-05	.1476E-02	.1877E+00
.6000E+02	.3076E-01	.3411E-01	.4991E-05	.1452E-02	.1877E+00
.6100E+02	.3076E-01	.3412E-01	.4991E-05	.1429E-02	.1877E+00
.6200E+02	.3076E-01	.3412E-01	.4992E-05	.1407E-02	.1877E+00
.6300E+02	.3076E-01	.3412E-01	.4992E-05	.1386E-02	.1877E+00
.6400E+02	.3076E-01	.3412E-01	.4992E-05	.1365E-02	.1877E+00
.6500E+02	.3076E-01	.3413E-01	.4993E-05	.1345E-02	.1877E+00
.6600E+02	.3076E-01	.3413E-01	.4993E-05	.1326E-02	.1877E+00
.6700E+02	.3076E-01	.3413E-01	.4993E-05	.1307E-02	.1877E+00
.6800E+02	.3076E-01	.3413E-01	.4994E-05	.1288E-02	.1877E+00
.6900E+02	.3076E-01	.3413E-01	.4994E-05	.1270E-02	.1877E+00
.7000E+02	.3076E-01	.3414E-01	.4994E-05	.1253E-02	.1877E+00
.7100E+02	.3076E-01	.3414E-01	.4994E-05	.1236E-02	.1877E+00
.7200E+02	.3076E-01	.3414E-01	.4995E-05	.1219E-02	.1877E+00
.7300E+02	.3076E-01	.3414E-01	.4995E-05	.1203E-02	.1877E+00
.7400E+02	.3076E-01	.3414E-01	.4995E-05	.1187E-02	.1877E+00
.7500E+02	.3076E-01	.3415E-01	.4995E-05	.1172E-02	.1877E+00
.7600E+02	.3076E-01	.3415E-01	.4996E-05	.1157E-02	.1877E+00
.7700E+02	.3076E-01	.3415E-01	.4996E-05	.1143E-02	.1877E+00
.7800E+02	.3076E-01	.3415E-01	.4996E-05	.1129E-02	.1877E+00
.7900E+02	.3076E-01	.3415E-01	.4996E-05	.1115E-02	.1877E+00
.8000E+02	.3076E-01	.3415E-01	.4996E-05	.1101E-02	.1877E+00
.8100E+02	.3076E-01	.3415E-01	.4997E-05	.1088E-02	.1877E+00
.8200E+02	.3076E-01	.3416E-01	.4997E-05	.1075E-02	.1877E+00
.8300E+02	.3076E-01	.3416E-01	.4997E-05	.1063E-02	.1877E+00
.8400E+02	.3076E-01	.3416E-01	.4997E-05	.1051E-02	.1877E+00
.8500E+02	.3076E-01	.3416E-01	.4997E-05	.1039E-02	.1877E+00
.8600E+02	.3076E-01	.3416E-01	.4998E-05	.1027E-02	.1877E+00
.8700E+02	.3076E-01	.3416E-01	.4998E-05	.1015E-02	.1877E+00
.8800E+02	.3076E-01	.3416E-01	.4998E-05	.1004E-02	.1877E+00
.8900E+02	.3076E-01	.3416E-01	.4998E-05	.9933E-03	.1877E+00
.9000E+02	.3076E-01	.3417E-01	.4998E-05	.9826E-03	.1877E+00
.9100E+02	.3076E-01	.3417E-01	.4998E-05	.9722E-03	.1877E+00
.9200E+02	.3076E-01	.3417E-01	.4999E-05	.9619E-03	.1877E+00
.9300E+02	.3076E-01	.3417E-01	.4999E-05	.9519E-03	.1877E+00
.9400E+02	.3076E-01	.3417E-01	.4999E-05	.9420E-03	.1877E+00
.9500E+02	.3076E-01	.3417E-01	.4999E-05	.9324E-03	.1877E+00
.9600E+02	.3076E-01	.3417E-01	.4999E-05	.9229E-03	.1877E+00
.9700E+02	.3076E-01	.3417E-01	.4999E-05	.9137E-03	.1877E+00
.9800E+02	.3076E-01	.3417E-01	.4999E-05	.9046E-03	.1877E+00
.9900E+02	.3076E-01	.3418E-01	.4999E-05	.8957E-03	.1877E+00

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  Model PlantX by Stefan Trapp
OrgC=0.665; CSoil=50 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:    .2290E+01 Henry:    .3970E+00 Halftime:    .2000E+01
  Equilibrium constants
   soil-water   :      .1193E+03
   air - soil   :      .3326E-02 air-water    :     .3970E+00
   root- soil   :      .1275E-01 root-water   :     .1522E+01
   leaves-soil  :      .4375E-01 leaves-water:      .5221E+01
   TSCF         :      .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :    .8278E-09 Metabolites:    .1469E-07 kg
 Amount in Stems :    .9619E-10 Metabolites:    .1743E-08 kg
 Amount in Leaves:    .1425E-09 Metabolites:    .2596E-08 kg
 Amount in Fruits:    .5376E-11 Metabolites:    .1798E-09 kg
 Conc. in Root   :    .6376E-06 Metabolites:    .1132E-04 kg/m3
 Conc. in Stem   :    .7088E-06 Metabolites:    .1284E-04 kg/m3
 Conc. in leaf   :    .3946E-06 Metabolites:    .7188E-05 kg/m3
 Conc. in fruit  :    .1840E-07 Metabolites:    .6153E-06 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :    .2059E-07 with transp. stream
 Uptake with water diff.:  -.3553E-10 air diff.    : -.5034E-08 kg
 Transport to leaves    :    .4716E-07 volatilised : -.4438E-07 kg
 Transport to stem      :    .4913E-07 to fruits   :   .1852E-09 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :   .6507E-09 m/s
```

OrgC=0.665; CSoil=50 ppb; CAir=30 ppt

Days	CRoot	CStem	CLeave	CFruit	CSoil
.0000E+00	.0000E+00	.0000E+00	.0000E+00	.0000E+00	.5000E-04
.1000E+01	.6376E-06	.6811E-06	.3946E-06	.1402E-06	.5000E-04
.2000E+01	.6376E-06	.6852E-06	.3946E-06	.1963E-06	.5000E-04
.3000E+01	.6376E-06	.6883E-06	.3946E-06	.2115E-06	.5000E-04
.4000E+01	.6376E-06	.6907E-06	.3946E-06	.2096E-06	.5000E-04
.5000E+01	.6376E-06	.6926E-06	.3946E-06	.2006E-06	.5000E-04
.6000E+01	.6376E-06	.6942E-06	.3946E-06	.1890E-06	.5000E-04
.7000E+01	.6376E-06	.6955E-06	.3946E-06	.1767E-06	.5000E-04
.8000E+01	.6376E-06	.6967E-06	.3946E-06	.1649E-06	.5000E-04
.9000E+01	.6376E-06	.6977E-06	.3946E-06	.1538E-06	.5000E-04
.1000E+02	.6376E-06	.6985E-06	.3946E-06	.1437E-06	.5000E-04
.1100E+02	.6376E-06	.6992E-06	.3946E-06	.1345E-06	.5000E-04
.1200E+02	.6376E-06	.6999E-06	.3946E-06	.1262E-06	.5000E-04
.1300E+02	.6376E-06	.7005E-06	.3946E-06	.1188E-06	.5000E-04
.1400E+02	.6376E-06	.7010E-06	.3946E-06	.1121E-06	.5000E-04
.1500E+02	.6376E-06	.7015E-06	.3946E-06	.1060E-06	.5000E-04
.1600E+02	.6376E-06	.7019E-06	.3946E-06	.1005E-06	.5000E-04
.1700E+02	.6376E-06	.7023E-06	.3946E-06	.9552E-07	.5000E-04
.1800E+02	.6376E-06	.7027E-06	.3946E-06	.9099E-07	.5000E-04
.1900E+02	.6376E-06	.7030E-06	.3946E-06	.8686E-07	.5000E-04
.2000E+02	.6376E-06	.7033E-06	.3946E-06	.8307E-07	.5000E-04
.2100E+02	.6376E-06	.7036E-06	.3946E-06	.7960E-07	.5000E-04
.2200E+02	.6376E-06	.7038E-06	.3946E-06	.7640E-07	.5000E-04
.2300E+02	.6376E-06	.7040E-06	.3946E-06	.7344E-07	.5000E-04
.2400E+02	.6376E-06	.7043E-06	.3946E-06	.7070E-07	.5000E-04
.2500E+02	.6376E-06	.7045E-06	.3946E-06	.6815E-07	.5000E-04
.2600E+02	.6376E-06	.7047E-06	.3946E-06	.6579E-07	.5000E-04
.2700E+02	.6376E-06	.7049E-06	.3946E-06	.6358E-07	.5000E-04
.2800E+02	.6376E-06	.7050E-06	.3946E-06	.6151E-07	.5000E-04
.2900E+02	.6376E-06	.7052E-06	.3946E-06	.5957E-07	.5000E-04
.3000E+02	.6376E-06	.7053E-06	.3946E-06	.5775E-07	.5000E-04
.3100E+02	.6376E-06	.7055E-06	.3946E-06	.5604E-07	.5000E-04
.3200E+02	.6376E-06	.7056E-06	.3946E-06	.5443E-07	.5000E-04
.3300E+02	.6376E-06	.7057E-06	.3946E-06	.5290E-07	.5000E-04
.3400E+02	.6376E-06	.7059E-06	.3946E-06	.5146E-07	.5000E-04
.3500E+02	.6376E-06	.7060E-06	.3946E-06	.5010E-07	.5000E-04
.3600E+02	.6376E-06	.7061E-06	.3946E-06	.4880E-07	.5000E-04
.3700E+02	.6376E-06	.7062E-06	.3946E-06	.4758E-07	.5000E-04
.3800E+02	.6376E-06	.7063E-06	.3946E-06	.4641E-07	.5000E-04
.3900E+02	.6376E-06	.7064E-06	.3946E-06	.4530E-07	.5000E-04
.4000E+02	.6376E-06	.7065E-06	.3946E-06	.4424E-07	.5000E-04
.4100E+02	.6376E-06	.7066E-06	.3946E-06	.4322E-07	.5000E-04
.4200E+02	.6376E-06	.7067E-06	.3946E-06	.4226E-07	.5000E-04
.4300E+02	.6376E-06	.7067E-06	.3946E-06	.4133E-07	.5000E-04
.4400E+02	.6376E-06	.7068E-06	.3946E-06	.4045E-07	.5000E-04
.4500E+02	.6376E-06	.7069E-06	.3946E-06	.3960E-07	.5000E-04
.4600E+02	.6376E-06	.7070E-06	.3946E-06	.3879E-07	.5000E-04
.4700E+02	.6376E-06	.7070E-06	.3946E-06	.3801E-07	.5000E-04
.4800E+02	.6376E-06	.7071E-06	.3946E-06	.3726E-07	.5000E-04
.4900E+02	.6376E-06	.7072E-06	.3946E-06	.3654E-07	.5000E-04
.5000E+02	.6376E-06	.7072E-06	.3946E-06	.3584E-07	.5000E-04
.5100E+02	.6376E-06	.7073E-06	.3946E-06	.3518E-07	.5000E-04
.5200E+02	.6376E-06	.7073E-06	.3946E-06	.3453E-07	.5000E-04
.5300E+02	.6376E-06	.7074E-06	.3946E-06	.3391E-07	.5000E-04
.5400E+02	.6376E-06	.7074E-06	.3946E-06	.3332E-07	.5000E-04
.5500E+02	.6376E-06	.7075E-06	.3946E-06	.3274E-07	.5000E-04
.5600E+02	.6376E-06	.7076E-06	.3946E-06	.3218E-07	.5000E-04
.5700E+02	.6376E-06	.7076E-06	.3946E-06	.3164E-07	.5000E-04

.5800E+02	.6376E-06	.7077E-06	.3946E-06	.3112E-07	.5000E-04
.5900E+02	.6376E-06	.7077E-06	.3946E-06	.3062E-07	.5000E-04
.6000E+02	.6376E-06	.7077E-06	.3946E-06	.3013E-07	.5000E-04
.6100E+02	.6376E-06	.7078E-06	.3946E-06	.2966E-07	.5000E-04
.6200E+02	.6376E-06	.7078E-06	.3946E-06	.2920E-07	.5000E-04
.6300E+02	.6376E-06	.7079E-06	.3946E-06	.2875E-07	.5000E-04
.6400E+02	.6376E-06	.7079E-06	.3946E-06	.2832E-07	.5000E-04
.6500E+02	.6376E-06	.7079E-06	.3946E-06	.2791E-07	.5000E-04
.6600E+02	.6376E-06	.7080E-06	.3946E-06	.2750E-07	.5000E-04
.6700E+02	.6376E-06	.7080E-06	.3946E-06	.2711E-07	.5000E-04
.6800E+02	.6376E-06	.7081E-06	.3946E-06	.2672E-07	.5000E-04
.6900E+02	.6376E-06	.7081E-06	.3946E-06	.2635E-07	.5000E-04
.7000E+02	.6376E-06	.7081E-06	.3946E-06	.2599E-07	.5000E-04
.7100E+02	.6376E-06	.7082E-06	.3946E-06	.2563E-07	.5000E-04
.7200E+02	.6376E-06	.7082E-06	.3946E-06	.2529E-07	.5000E-04
.7300E+02	.6376E-06	.7082E-06	.3946E-06	.2496E-07	.5000E-04
.7400E+02	.6376E-06	.7083E-06	.3946E-06	.2463E-07	.5000E-04
.7500E+02	.6376E-06	.7083E-06	.3946E-06	.2432E-07	.5000E-04
.7600E+02	.6376E-06	.7083E-06	.3946E-06	.2401E-07	.5000E-04
.7700E+02	.6376E-06	.7083E-06	.3946E-06	.2371E-07	.5000E-04
.7800E+02	.6376E-06	.7084E-06	.3946E-06	.2341E-07	.5000E-04
.7900E+02	.6376E-06	.7084E-06	.3946E-06	.2312E-07	.5000E-04
.8000E+02	.6376E-06	.7084E-06	.3946E-06	.2285E-07	.5000E-04
.8100E+02	.6376E-06	.7084E-06	.3946E-06	.2257E-07	.5000E-04
.8200E+02	.6376E-06	.7085E-06	.3946E-06	.2231E-07	.5000E-04
.8300E+02	.6376E-06	.7085E-06	.3946E-06	.2205E-07	.5000E-04
.8400E+02	.6376E-06	.7085E-06	.3946E-06	.2179E-07	.5000E-04
.8500E+02	.6376E-06	.7085E-06	.3946E-06	.2154E-07	.5000E-04
.8600E+02	.6376E-06	.7086E-06	.3946E-06	.2130E-07	.5000E-04
.8700E+02	.6376E-06	.7086E-06	.3946E-06	.2106E-07	.5000E-04
.8800E+02	.6376E-06	.7086E-06	.3946E-06	.2083E-07	.5000E-04
.8900E+02	.6376E-06	.7086E-06	.3946E-06	.2060E-07	.5000E-04
.9000E+02	.6376E-06	.7086E-06	.3946E-06	.2038E-07	.5000E-04
.9100E+02	.6376E-06	.7087E-06	.3946E-06	.2016E-07	.5000E-04
.9200E+02	.6376E-06	.7087E-06	.3946E-06	.1995E-07	.5000E-04
.9300E+02	.6376E-06	.7087E-06	.3946E-06	.1974E-07	.5000E-04
.9400E+02	.6376E-06	.7087E-06	.3946E-06	.1954E-07	.5000E-04
.9500E+02	.6376E-06	.7087E-06	.3946E-06	.1934E-07	.5000E-04
.9600E+02	.6376E-06	.7087E-06	.3946E-06	.1914E-07	.5000E-04
.9700E+02	.6376E-06	.7088E-06	.3946E-06	.1895E-07	.5000E-04
.9800E+02	.6376E-06	.7088E-06	.3946E-06	.1876E-07	.5000E-04
.9900E+02	.6376E-06	.7088E-06	.3946E-06	.1858E-07	.5000E-04

```
 Model PlantX by Stefan Trapp
Meadow Park Spring:CSoil=18.5 ppb; CAir=30 ppt
 MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
 Equilibrium constants
  soil-water  :       .9287E+01
  air - soil  :       .4275E-01 air-water   :    .3970E+00
  root- soil  :       .1639E+00 root-water  :    .1522E+01
  leaves-soil :       .5621E+00 leaves-water:    .5221E+01
  TSCF        :       .7047E+00
Simulation run time (days) :    .1000E+03
Amount in Roots :    .3936E-08 Metabolites:   .6985E-07 kg
Amount in Stems :    .4571E-09 Metabolites:   .8279E-08 kg
Amount in Leaves:    .1426E-09 Metabolites:   .2598E-08 kg
Amount in Fruits:    .2555E-10 Metabolites:   .8536E-09 kg
Conc. in Root   :    .3031E-05 Metabolites:   .5380E-04 kg/m3
Conc. in Stem   :    .3369E-05 Metabolites:   .6101E-04 kg/m3
Conc. in leaf   :    .3950E-06 Metabolites:   .7195E-05 kg/m3
Conc. in fruit  :    .8743E-07 Metabolites:   .2921E-05 kg/m3
Total Transpiration m3 :   .1664E+00 phloem flux :  .6560E-03 m3
Uptake into roots      :   .9788E-07 with transp. stream
Uptake with water diff.:  -.1689E-09 air diff.   : -.2394E-07 kg
Transport to leaves    :   .2240E-06 volatilised : -.2213E-06 kg
Transport to stem      :   .2336E-06 to fruits   :  .8792E-09 kg
Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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  Model PlantX by Stefan Trapp
Omer Well:CSoil=11.5 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:   .2290E+01 Henry:    .3970E+00 Halftime:    .2000E+01
  Equilibrium constants
   soil-water  :      .9287E+01
   air - soil  :      .4275E-01 air-water    :     .3970E+00
   root- soil  :      .1639E+00 root-water   :     .1522E+01
   leaves-soil :      .5621E+00 leaves-water:      .5221E+01
   TSCF        :      .7047E+00
 Simulation run time (days) :    .1000E+03
 Amount in Roots :   .2447E-08 Metabolites:    .4342E-07 kg
 Amount in Stems :   .2842E-09 Metabolites:    .5147E-08 kg
 Amount in Leaves:   .1426E-09 Metabolites:    .2597E-08 kg
 Amount in Fruits:   .1588E-10 Metabolites:    .5307E-09 kg
 Conc. in Root   :   .1884E-05 Metabolites:    .3345E-04 kg/m3
 Conc. in Stem   :   .2094E-05 Metabolites:    .3793E-04 kg/m3
 Conc. in leaf   :   .3948E-06 Metabolites:    .7192E-05 kg/m3
 Conc. in fruit  :   .5435E-07 Metabolites:    .1816E-05 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :   .6084E-07 with transp. stream
 Uptake with water diff.:  -.1050E-09 air diff.    : -.1488E-07 kg
 Transport to leaves    :   .1393E-06 volatilised : -.1365E-06 kg
 Transport to stem      :   .1452E-06 to fruits    :  .5466E-09 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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  Model PlantX by Stefan Trapp
Sunset Drain:CSoil=6.3 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:   .2290E+01 Henry:    .3970E+00 Halftime:    .2000E+01
  Equilibrium constants
   soil-water  :      .9287E+01
   air - soil  :      .4275E-01 air-water   :     .3970E+00
   root- soil  :      .1639E+00 root-water  :     .1522E+01
   leaves-soil :      .5621E+00 leaves-water:     .5221E+01
   TSCF        :      .7047E+00
 Simulation run time (days) :    .1000E+03
 Amount in Roots :    .1340E-08 Metabolites:   .2379E-07 kg
 Amount in Stems :    .1557E-09 Metabolites:   .2820E-08 kg
 Amount in Leaves:    .1425E-09 Metabolites:   .2596E-08 kg
 Amount in Fruits:    .8702E-11 Metabolites:   .2909E-09 kg
 Conc. in Root   :    .1032E-05 Metabolites:   .1832E-04 kg/m3
 Conc. in Stem   :    .1147E-05 Metabolites:   .2078E-04 kg/m3
 Conc. in leaf   :    .3947E-06 Metabolites:   .7189E-05 kg/m3
 Conc. in fruit  :    .2978E-07 Metabolites:   .9955E-06 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :   .3333E-07 with transp. stream
 Uptake with water diff.:  -.5752E-10 air diff.   : -.8151E-08 kg
 Transport to leaves    :   .7632E-07 volatilised : -.7354E-07 kg
 Transport to stem      :   .7955E-07 to fruits   :  .2996E-09 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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```
  Model PlantX by Stefan Trapp
Martin Spring:CSoil=6.2 ppb; CAir=30 ppt
  MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:    .2000E+01
  Equilibrium constants
   soil-water  :       .9287E+01
   air - soil  :       .4275E-01 air-water   :     .3970E+00
   root- soil  :       .1639E+00 root-water  :     .1522E+01
   leaves-soil :       .5621E+00 leaves-water:     .5221E+01
   TSCF        :       .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :   .1319E-08 Metabolites:   .2341E-07 kg
 Amount in Stems :   .1532E-09 Metabolites:   .2776E-08 kg
 Amount in Leaves:   .1425E-09 Metabolites:   .2596E-08 kg
 Amount in Fruits:   .8564E-11 Metabolites:   .2863E-09 kg
 Conc. in Root   :   .1016E-05 Metabolites:   .1803E-04 kg/m3
 Conc. in Stem   :   .1129E-05 Metabolites:   .2045E-04 kg/m3
 Conc. in leaf   :   .3947E-06 Metabolites:   .7189E-05 kg/m3
 Conc. in fruit  :   .2931E-07 Metabolites:   .9797E-06 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :   .3280E-07 with transp. stream
 Uptake with water diff.:  -.5661E-10 air diff.   : -.8022E-08 kg
 Transport to leaves    :   .7511E-07 volatilised : -.7233E-07 kg
 Transport to stem      :   .7829E-07 to fruits   :  .2948E-09 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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  Model PlantX by Stefan Trapp
Meadow Park Drain:CSoil=2.8 ppb; CAir=30 ppt
  MW:    .1314E+03 logKow:    .2290E+01 Henry:    .3970E+00 Halftime:    .2000E+01
  Equilibrium constants
   soil-water   :       .9287E+01
   air - soil   :       .4275E-01 air-water    :     .3970E+00
   root- soil   :       .1639E+00 root-water   :     .1522E+01
   leaves-soil  :       .5621E+00 leaves-water:      .5221E+01
   TSCF         :       .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :    .5957E-09 Metabolites:    .1057E-07 kg
 Amount in Stems :    .6923E-10 Metabolites:    .1254E-08 kg
 Amount in Leaves:    .1425E-09 Metabolites:    .2596E-08 kg
 Amount in Fruits:    .3869E-11 Metabolites:    .1295E-09 kg
 Conc. in Root   :    .4588E-06 Metabolites:    .8143E-05 kg/m3
 Conc. in Stem   :    .5102E-06 Metabolites:    .9244E-05 kg/m3
 Conc. in leaf   :    .3946E-06 Metabolites:    .7188E-05 kg/m3
 Conc. in fruit  :    .1324E-07 Metabolites:    .4430E-06 kg/m3
 Total Transpiration m3 :    .1664E+00 phloem flux :   .6560E-03 m3
 Uptake into roots      :    .1481E-07 with transp. stream
 Uptake with water diff.:   -.2557E-10 air diff.    : -.3623E-08 kg
 Transport to leaves    :    .3395E-07 volatilised : -.3117E-07 kg
 Transport to stem      :    .3536E-07 to fruits    :  .1333E-09 kg
 Conductivity of Stomata:    .8544E-03 of Cuticula :  .6507E-09 m/s
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  Model PlantX by Stefan Trapp
Chicado Well:CSoil=2.3 ppb; CAir=30 ppt
  MW:   .1314E+03 logKow:   .2290E+01 Henry:   .3970E+00 Halftime:   .2000E+01
  Equilibrium constants
   soil-water  :     .9287E+01
   air - soil  :     .4275E-01 air-water    :    .3970E+00
   root- soil  :     .1639E+00 root-water   :    .1522E+01
   leaves-soil :     .5621E+00 leaves-water:     .5221E+01
   TSCF        :     .7047E+00
 Simulation run time (days) :     .1000E+03
 Amount in Roots :   .4893E-09 Metabolites:   .8684E-08 kg
 Amount in Stems :   .5688E-10 Metabolites:   .1031E-08 kg
 Amount in Leaves:   .1425E-09 Metabolites:   .2595E-08 kg
 Amount in Fruits:   .3179E-11 Metabolites:   .1064E-09 kg
 Conc. in Root   :   .3769E-06 Metabolites:   .6689E-05 kg/m3
 Conc. in Stem   :   .4191E-06 Metabolites:   .7596E-05 kg/m3
 Conc. in leaf   :   .3946E-06 Metabolites:   .7188E-05 kg/m3
 Conc. in fruit  :   .1088E-07 Metabolites:   .3641E-06 kg/m3
 Total Transpiration m3 :   .1664E+00 phloem flux :  .6560E-03 m3
 Uptake into roots      :   .1217E-07 with transp. stream
 Uptake with water diff.:  -.2100E-10 air diff.    : -.2976E-08 kg
 Transport to leaves    :   .2789E-07 volatilised : -.2512E-07 kg
 Transport to stem      :   .2904E-07 to fruits    :  .1096E-09 kg
 Conductivity of Stomata:   .8544E-03 of Cuticula :  .6507E-09 m/s
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13. ABSTRACT *(Maximum 200 words)*

This research expands our limited knowledge on the influence of plants on the fate and effects of trichloroethylene (TCE), providing a screening tool on which to base decisions regarding the need for actual sampling of plants. First, physicochemical properties of TCE--vapor pressure, Henry's Law constant, water solubility, octanol-water partition coefficient, molecular weight, and half-life--were screened against relationships reported in literature to evaluate TCE plant uptake potential. This screening approach indicated TCE may be transferred to plants via retention by root surfaces, root uptake and translocation, and foliar uptake. Next, the PLANTX model developed by Trapp and others was applied to a representation of a soybean plant to determine minimum soil TCE concentrations which result in plant TCE levels exceeding 5 micrograms per liter of solution (ug/L). The simulations indicated that stem and root crops are most susceptible to TCE uptake and accumulation, while significantly higher soil and air TCE concentrations are required to produce leaf and fruit TCE levels of concern to human health. The above procedures were then applied to an off-site contamination situation near Hill Air Force Base, Utah. The simulations indicate that existing TCE concentrations in irrigation water from contaminated residential wells and springs do not result in plant TCE levels greater than 5 ug/L.

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